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# Pushing the boundaries of technology to educate and train the next generation of crystallographers

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This article describes the evolution of educational technologies, moving from the Web 1.0 to the current Web 3.0 decade, with the aim of stimulating discussion and inspiring innovative and effective crystallography education in the Web 3.0 decade. In the last 15 years, academic crystallography has largely migrated from a research specialty to a technique employed by a broad user community. This has led to the growth of and dependence on independently funded workshops and summer schools, as well as other non-traditional curricular resources for crystallography instruction, such as web pages and online courses, which allow crystallography to be self-taught. In fact, informal courses and e-learning constitute 70-80% of all learning today, and students expect on-demand learning. Implementing modern web technologies with sound pedagogy requires skilful integration of relevant, often disparate, resources into useful and usable frameworks, enabling learners to interact, explore new situations, and use scientific reasoning skills such as hypothesis testing and model-based reasoning. The evident disproportion in implementing contemporary technologies into our global crystallography education resources requires that we shift our focus from simply imparting subject knowledge by posting largely text-based content to empowering students with the fundamental processes and skills needed for ondemand learning and practice in crystallography.

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### 1. Cyberinfrastructure and e-learning

'The future is already here, it's just unevenly distributed.'

So said William Gibson, American science fiction writer, in 1999 (interview on NPR radio station, 30 November 1999). The future in the present context of this article is cyberinfrastructure, and its impact on crystallography education and training in the Web 3.0 decade. Cyberinfrastructure is the coordinated aggregate of software, hardware and other technologies, as well as human expertise, required to support current and future discoveries in science and engineering (Cyberinfrastructure Council, 2007). Rapid advances in networking, web-based tools and other aspects of cyberinfrastructure may be exploited by researchers and educators to facilitate broader access to instrumentation and achieve broader impact (Kantardjieff & Lifton, 2008). The challenge of cyberinfrastructure is to integrate relevant and often disparate resources to provide a useful, usable and enabling framework for research, discovery and education characterized by broad access and 'end-to-end' coordination (Berman & Brady, 2005).

We have now entered the Web 3.0 decade, moving beyond dynamic and shared web content to semantically integrated information and collective intelligence. Yet the use of cyberinfrastructure to effectively connect data, computers and people in pedagogically sound ways is certainly unevenly distributed across universities, research institutes and industries. This is due partly to legitimate technological naïveté by those who did not grow up with it or train with it professionally, and partly to scepticism about cyberinfrastructure, its 'robustness' and the synergistic relationship it has with modern society.

The reality today is that informal courses and e-learning constitute 70–80% of our learning, and it has been proposed that standard courses with pre-packaged curricula are indeed dead (Cross, 2007). Instead, students today expect on-demand learning, where one might download the necessary materials when a problem or situation arises. Among higher education students, 17% are enrolled in online curricula (Whittaker, 2009), 60% belong to a social network, 75% regularly use a laptop computer, 85% say technology is an important tool for their field of chosen study and 39% rate online chatting with instructors as the most useful technology in their studies (CDW-G, 2008). Students also recommend the use of videos, instructional web sites, slide shows, wikis and online experiments to better instruct and familiarize them with relevant information (CDW-G, 2008).

Remotely controlled (cyber-enabled) scientific instrumentation is becoming an integral part of performing scientific research, providing access to unique and/or expensive instrumentation without requiring the user to be physically present, facilitating collaboration, consultation and distributed expertise, and affording exceptional opportunities for education and training. Computer simulations create scenarios where learners are given tasks that embody the kinds of knowledge and skills they will need in the real situation. Effective simulations embed cognitive skills and knowledge in the kinds of contexts they will be applied, so that learners not only gain competency, but also appreciate when and how to apply those competencies. Simulations can also allow learners to try different courses of action, asking 'What if?' questions, exploring different solutions and experiencing different contingencies. When simulations become 'serious games', learners take on roles that enable them to interact with one another, shape the environment and explore new situations, as well as use scientific reasoning skills, including hypothesis testing and revision, and model-based reasoning (Steinkuehler, 2008).

To create and prepare such cyber-enabled online environments and experiences in educational contexts, it is unwise and pedagogically deadly simply to port content from a traditional course to the on-demand environment. Information content is assimilated and integrated quite differently in the online environment, and there is a great need for sound pedagogy, using the growing number of technologies and delivery mechanisms to facilitate learning in the Web 3.0 decade. For example, one might rely on asynchronous technologies, such as discussion boards and practice exams, which allow for flexibility in work schedules and are relatively insensitive to temporal and geographical constraints. In another context, synchronous communications, such as real-time chats, webinars, video conferencing and remotely enabled instruments, facilitate greater interaction with an instructor or expert, as well as immediate feedback to participants' questions and concerns. Blended learning environments combine the best of these worlds.

# **1.1.** The role of cyberinfrastructure in crystallography education and training

So, what does this all have to do with crystallography education and training? There is a growing concern, particularly in the USA, that education in general is neither training adequate numbers of students for careers in science and technology, nor developing the broad scientific and technological literacy that is necessary for full participation in society. In our own field of crystallographic science, we have seen highprofile and embarrassing retractions in the peer-reviewed literature, many the result of pathological science or inadequate review (Dauter & Baker, 2010; Harrison *et al.*, 2010).

In the past 15 years, academic crystallography has largely migrated from a research specialty to a technique employed by a wide community of users. As a consequence, few university departments in the USA hire faculty capable of teaching crystallography, and formal courses have all but disappeared from course catalogues. However, increasingly large numbers of 'naïve' users (Cassman, 1999), who require more assistance than the experienced user, work in academia and industry. This has led to the growth of and dependence on independently funded workshops and summer schools in crystallography, aimed at different audiences, as well as an increasing dependence on other, non-traditional, curricular resources for instruction, such as web pages and, more recently, online courses, which allow crystallography to be self-taught.

Web-based tutorials can afford an extremely valuable resource to the broader scientific community, provided they are pedagogically well constructed and not merely electronic file cabinets of lecture notes and slide presentations. While the static web pages of Web 1.0 could not provide practical experience, the dynamic content of Web 2.0 facilitates practice and collaboration. The connectivity of Web 2.0 and the integration of information in Web 3.0 can now provide practical experience through live, remote-enabling and realistic virtual environments, as well as transmit the fascination and excitement of the field necessary to attract a future generation of professional crystallographers. As noted by the United States National Committee for Crystallography in its education and training policies white paper, 'There is common ground in the fundamental physics of crystallography shared by scientists in the life sciences and by those in the physical sciences, but the objectives of each community in applying crystallography to their particular research problems are not necessarily the same... If the science of crystallography is to remain alive and vibrant, it is critical that crystallography be taught in a way that attracts and retains a broad pool of talented people.' (USNCCr and ACA, 2006).

## 2. Web 2.0 and beyond

Web 2.0 is a collection of tools and technologies enabling people who access the internet, consume media and use the web to do more than passively absorb what is presented. These tools enable people actively to contribute to and customize content through the use of blogs, wikis, social networking applications, RSS (really simple syndication) feeds, podcasts, collaboration webs and massively multiplayer online gaming applications (Fig. 1). Although some of these tools were not originally intended for instruction, they have been shown to be extremely effective in facilitating learning by the digital generation. Increasing numbers of educators use blogs, podcasts, wikis and Twitter as additional approaches to achieve effective learning. YouTube began as a video-sharing web site where users upload and share video content. In 2009, YouTube released a new subsite called YouTube EDU, which aggregates thousands of free lectures from over 100 universities across the US, including MIT, Yale, Harvard and Stanford, and around the world, and currently offers more than 200 full courses on demand (Fig. 2). iTunes U is another innovative and powerful online distribution system of educational content, supporting multiple media formats and enabling learning on demand and customized learning. Educational content, including more than 250 000 lectures from around the world, is available from more than 600 universities, as well as museums, libraries and other cultural institutions from 'beyond campus'.

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If Web 1.0 was the web as an information portal (read-only), and Web 2.0 was a platform for creating and validating information (wildly read-write), then Web 3.0 is about organizing information (semantic), personalizing information (contextualizing) and extracting meaning from the way we interact with information (artificial intelligence). Also, it is highly mobile (on demand). Examples of this kind of information integration now available (data mashups) are iGoogle, Netvibes and StumbleUpon. Imagine having a homepage that personalizes information content (iGoogle or Netvibes) by subscribing to various online media services, and uses an embedded application (StumbleUpon) to make personal recommendations for you about content having to do with crystallography. Further, you would have all the content, tailored to your personal learning needs, available on-demand from your Blackberry, Droid or iPhone/iPod/iPad.

When we consider the use of these robust tools to facilitate contemporary learning and training, we must realize that it is no longer about the technology itself, how to use it, but rather about its impact, how it is used (Rychen, 2002). Today, people are at the center of the information space, which is profoundly influencing how we relate to knowledge and information, the way we do research and evaluate credibility, and the manner by which we learn to be professionals in our chosen discipline. While there is certainly the risk that collective intelligence, *i.e.* new forms of information stores gathered collaboratively or competitively by many people, can quickly become collective ignorance, the new reality suggests that books, posted lecture notes, slide presentations and static web pages may no longer be as valuable for contemporary learning as they once were, given the contemporaneous nature of blogs, wikis, RSS feeds and streaming video. Generations Y and Z (students) consider e-mail passé (Whittaker, 2009). Perhaps the written word has begun to exceed its usefulness in some learning contexts. Experts agree that, in the new virtual classroom of the internet, effective visual treatments support learning by

facilitating attention, activation of prior knowledge, management of cognitive load, building of new mental models, transference of learning and motivation (Colvin-Clark & Kwinn, 2007). The process of learning also involves making decisions, taking an action and receiving feedback, features manifest in online simulations and gaming.

# 3. Cyber-enabled instrumentation provides practical experience

Cyber-enabled instrumentation is clearly becoming an integral part of performing scientific research. I cite my own humble beginnings as a graduate student at UCLA in the early 1980s, working in David Eisenberg's laboratory. Our diffractometers were computer controlled, and computers were remotely accessible via dial-up modem. Data files, showing whether data with good signal-to-noise were being collected, as well as instrument status, could be monitored entirely by command line entries. Since 1994 (Goldberg et al., 2000), remote instrumentation access has been an increasingly viable option for conducting experiments, and it has been applied in an educational context by universities in undergraduate engineering fields since 1996 (Aktan et al., 1996). Moreover, what and how students learned using these technologies has been assessed. Remote control of instruments is not necessarily an inferior pedagogy, as it tends to emphasize experimental design and problem-solving.

Crystallography was one of the first scientific areas to implement remote instrumentation access successfully and to benefit from 'collaboratories' (Carragher & Potter, 1999). Pilot studies were started in the late 1990s between NRCC, SSRL and CHESS to accept mailed samples for remote access and control of beamlines over the internet (Cassman, 1999). Today, many synchrotron beamlines are remotely enabled and researchers, including undergraduate and graduate students, routinely engage in remote data collection (Kantardjieff, 2009). In late 1997, the Keck Center for Molecular Structure (CMolS), the first facility of its kind in the undergraduate environment, pioneered the use of remotely enabled instru-



Figure 1

Social media as we move into the Web 3.0 decade. Social networks, features and functionalities of Web 2.0/3.0, and the purposes they can serve in crystallography education and training.



#### Figure 2

YouTube EDU. Seeing Bonds by Electron Difference Density from Yale Courses. Note that this is closed-captioned and compliant with disability laws in the USA, which deal with and oversee accessibility.

ments for undergraduate research and training in the California State University (Kantardjieff, 1999). Other predominantly undergraduate institutions soon followed our lead. In 2005, Allen Hunter at Youngstown State University established the STaRBURSTT CyberDiffraction Consortium, a national network of faculty with teaching and research interests in crystallography, supported by remotely enabled diffraction facilities at five institutions (Hunter *et al.*, 2005).

Interest in remote scientific instrumentation projects for K-12 (kindergarten through 12th grade) education is growing, first prompted in a 1997 memorandum by US President Clinton, in which he emphasized enriching the role of the internet as a learning and teaching resource (Clinton, 1997). Despite the growing importance of remote instrumentation, educational projects have been slow to incorporate its use for pre-college instruction. However, with the advance of browser-based graphical user interfaces and commercial offthe-shelf applications, curricula are changing and consortia are active. An excellent example of how remote enabling has successfully percolated to the K-12 regime is 'The Bugscope Project' (http://bugscope.beckman.illinois.edu/), launched in 1999. Bugscope is an educational outreach project of the World Wide Laboratory, giving K-12 teachers free access to a \$600 000 scanning electron microscope via the internet, and thus bringing the classroom to the microscope. Students collect bugs and send them to the facility where they are mounted by staff. At the scheduled time, students log on over the internet, viewing their specimen and chatting with Bugscope staff, together describing, seeing and answering questions in real-time. A more recent project is CAL-PRISSM (Kantardjieff et al., 2007), an e-science consortium supported by The Boeing Company, providing its members from several predominantly undergraduate institutions, community colleges and high schools with real-time remote access and control of specialized scientific instruments from remote locations (including diffractometers, resonance spectrometers, mass spectrometers and an array of microscopes), together with real-time discourse. CAL-PRISSM aims not only to promote cross-disciplinary collaboration between researchers using these technologies, but also to improve educational quality and student opportunities at the undergraduate and secondary levels in learning about and researching the structure of matter. Members design, deploy and assess learning units and simulations that address California State University Programmatic Student Learning Outcomes and the California Science Content Standards with regard to various aspects of the structure of matter.

# 4. Virtual environments make possible new models of learning

A number of colleges and universities around the world have built virtual classrooms in Second Life, an online environment where people interact with the environment and each other *via* avatars (from the Sanskrit word for 'a form of self', a computer user's representation of himself/herself or *alter ego*). Because online education can seem foreign to instructors trained in physical classrooms, initial efforts to build virtual worlds tried to make them look like regular classrooms. Unfortunately, and speaking from personal experience, moving around in Second Life can be rather cumbersome, and many instructors and students have decided that there are far easier ways to interact when they are geographically and temporally distributed.

Virtual environments and simulations, however, show great promise pedagogically, particularly in the form of serious online gaming. In this context, we find that virtual worlds enable instructors to stage medical simulations, guide students through the inside of cell structures, conduct virtual laboratories and safety training, or present other imaginative teaching exercises that cannot practicably be done in a physical environment. Utilizing virtual laboratory environments to educate and train students in crystallographic science has great potential to provide safe, engaging and practical hands-on experience without the need to be proximal to or usurp an instrument. At the same time, virtual laboratory environments can still facilitate collaboration, consultation and distributed expertise.

An example of a successful virtual scientific training implementation has been created at Brigham Young University. 'Y Science Laboratories' is a set of sophisticated and realistic simulations dealing with biology, chemistry, physical science, physics and earth science (http://chemlab.byu.edu). In virtual environments, students are presented with case studies, where they make decisions as they would in a real laboratory and experience the consequences. Another example is the Virtual Environments for Safety Training Laboratory (VEST-Lab), created by a post-graduate student at the University of Sussex. VEST-Lab realistically reproduces a three-dimensional chemistry laboratory, in which participants navigate their way around looking out for potential hazards and responding to emergency scenarios (Perez & Cox, 2009). A third example is the University of Cincinnati's virtual Galapagos Islands (http://www.uc.edu/darwin/). Opened in 2009 to celebrate the 150th anniversary of Charles Darwin's On the Origin of Species, the virtual Galapagos allow anyone with internet access and a machine capable of running the Second Life software to visit the islands, learn about Darwin's work and the ecology of the Galapagos, and virtually attend symposia and lectures streamed live from the University of Cincinnati campus and from regional partner organizations.

An entire university can be created in the virtual world as well. Founded by Royal Charter in 1969, the Open University (OU) is the largest university in the United Kindgom (http:// www.open.ac.uk/). Dedicated to providing quality distance education, the OU allows students flexibility to learn with its extended virtual world campus in Second Life. Here, workers can train in a cost-effective manner to manage combat or natural disaster, and students can earn a BSc in Molecular Science.

Supporting broader efforts, the Immersive Education Initiative (iED) is a merit-based non-profit international collaboration of higher education institutions, research institutes, companies and consortia, founded by Aaron E. Walsh, a

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professor of advancing studies at Boston College (http:// immersiveeducation.org). iED members work together to define and develop open standards, best practices and platforms, and to support communities for virtual reality and game-based learning and training. Using the 'Education Grid', iED members conduct classes and meetings in virtual worlds, as well as build custom virtual-learning worlds, simulations and learning games.

# 5. Online and distance learning transcend boundaries in crystallography

Let us look at just a few examples of effective online and distance learning implementations over the years, specifically in crystallography, highlighting the cyberinfrastructure utilized. This is not intended to be a definitive list, as there have been numerous online tutorials and course content made available during the Web 1.0 and Web 2.0 decades, some of which are described elsewhere in this issue. The examples in this article have been selected because they utilized the sophisticated and emerging technology available at the time of their creation and implementation, both asynchronously and synchronously, and included remotely enabled instruments. They also considered pedagogy and the evolving educational environment, and did not simply port existing lecture content from a traditional course.

*Crystallography 101* (http://www.ruppweb.org) was launched by Bernhard Rupp in 1993 when the World Wide Web was still quite new (Web 1.0) and was composed mainly of static pages. The cutting-edge technologies of the day included the NCSA *Mosaic* browser and Windows NT 3.0. What distinguished this X-ray tutorial from anything else on the web was not only its content, but its effective use of interactive graphics and exercises. These pages have been utilized by more than half a million people worldwide as a valuable resource for on-demand learning. Although the pages are still active and the content quite useful, new pages will appear as part of a new tutorial based on Web 3.0 technologies accompanying a new book, *Biomolecular Crystallography*, information about which can be found on Facebook (*Biomolecular Crystallography – The Book*).

*e-Crystallography* (http://escher.epfl.ch/eCrystallography/) is an interactive course in crystallography for the presentation of basic crystallography concepts, developed by Gerard Chapuis at the École Polytechnique Fédérale de Lausanne. Like *Crystallography 101, e-Crystallography* presents extensive content as a mix of static web pages coupled with interactive exercises and applets. It also incorporates Web 2.0 tools, such as user groups and discussion forums.

*Molecular and Solid State Physics* is a course web site maintained by Peter Hadley (http://lamp.tu-graz.ac.at/ ~hadley/ss1/introduction/index.php), Technical University of Graz. What is noteworthy about this web site is neither its format nor its archiving of lectures. It is well organized and makes modest use of animations. However, the instructor actively engages students in the learning process by having them contribute to the course, both its content and its dissemination. Students create and produce video projects, designed to improve course content, while also casting it in a fundamental media type for all content on the web. Thus, at the same time as they learn about solid-state physics, students learn to use important Web 2.0 communication tools.

*CCP4 Wiki* (http://ccp4wiki.org) is a repository of knowledge and documentation for *CCP4* users and crystallographers, which provides background for using the *CCP4* suite of programs (Collaborative Computational Project, Number 4, 1994). Associated resources include a 'crystallographic knowledge base', such as a glossary of terms, steps in the structure-solution process, and lectures and presentations from various workshops. Because this is a wiki, it supports facile creation and editing of interlinked web pages. It is an example of Web 2.0 collective intelligence that emerges from networking and collaboration among a virtual community of individuals coming together with shared interests and a common purpose.

*P212121* (http://www.p212121.com/) is a recent addition to the battery of crystallographic resources utilizing Web 2.0/3.0 technologies. P212121 is a blog, the goal of which is to provide a platform for the crystallographic community to share ideas. P212121 takes advantage of social networking applications such as Twitter, Facebook and RSS feeds to distribute content across the web. Individuals subscribe to these feeds, capturing them within the applications themselves, or using tools designed to capture feeds, such as Outlook, Google Reader and Yoono. An increasing number of educators use RSS feeds to stay in contact with and inform distance-learning students, as well as to drive and moderate online learning discourse.

*YouTube EDU* (http://www.youtube.com/education?b=400) currently offers 60 video lectures on topics in crystallography, mainly series from MIT and Yale University, but also including award lectures by David Eisenberg and Thomas Steitz.

iTunes U (http://www.apple.com/education/itunes-u/) currently offers about a dozen crystallography selections from five universities worldwide, covering organic chemistry, biochemistry and guided drug-discovery applications, both audio and video.

*Birkbeck College* (http://www.cryst.bbk.ac.uk/) has offered advanced online courses in crystallography for several years, and currently offers both MSc and postgraduate certificates through distance learning. Instruction utilizes asynchronous communication *via* web pages for presenting course content, and email for submission of questions and completed assignments. Tutorials and interactive sessions utilize synchronous communications in virtual environments similar to chat rooms. Because the courses are taught online and in modular format, they allow students great flexibility in their study patterns. This is of particular importance as increasing numbers of postbaccalaureate students study part-time.

*Practical X-ray Crystallography* is an undergraduate course at California State University Fullerton. Because crystallography courses are rarely offered in the undergraduate curriculum in the USA, what has distinguished this course has been its synchronous delivery to other campuses over the past decade, beginning in 1997, when we taught this course jointly with San Jose State University (400 miles north of Fullerton). While lecture materials were posted on the web, SJSU students remotely controlled instruments at CMolS to collect and analyze data from samples they had sent by post. This was achieved with a commercial off-the-shelf product called *pcAnywhere*, running under DOS.

In 2007, we taught this course jointly with Harvey Mudd College, 15 miles from Fullerton, utilizing a variety of Web 2.0 tools to advance learning (Kantardjieff, 2007). Lectures were delivered by instructors on two separate campuses to students on both campuses using the *iLinc* web conferencing suite (institutional licensing). LogMeIn remote-access and desktop software (free version) provided connectivity to quickly establish and verify data collection on instruments. Pando (free peer-to-peer software) was utilized for sending, sharing and downloading large data files across campus firewalls. Laboratory demonstrations were streamed live using web cameras and recorded for later viewing as podcasts. Video tutorials on the use of various software suites were also podcast. Lecture presentations were recorded, both video and audio, using *iLinc*, *SnapKast* (modest academic licensing), Camtasia Studio (modest academic licensing) or the opensource CamStudio (free). Interactive sessions, tutorials and office hours utilized synchronous communications via iLinc, with voice over internet protocol (VoIP) and live chatting. Shared desktops facilitated collaboration and consultation and distributed expertise while students worked on their individual structure projects. Course materials, including recorded class sessions and discussion boards, were distributed through each campus' course-management system, opensource Sakai (educational community license) or Blackboard (institutional licensing). Today, many of these activities could be achieved easily and at no cost with Moodle (http:// moodle.org).

Modern Biomolecular Crystallography and Crystallography for Chemists are workshops we have conducted at CMolS through the Center for Workshops in Chemical Sciences (http://chemistry.gsu.edu/CWCS), sponsored by the National Science Foundation. The goals of these workshops, which are aimed primarily at faculty from two- and four-year colleges and universities in the USA, are to provide background and a modern perspective on key areas of the chemical sciences, and to suggest pedagogically sound methods to introduce these topics into the undergraduate curriculum. During our most recent workshop in 2008, facilitators' presentations were delivered to remote participants using *iLinc* and recorded for post-workshop viewing. The workshop curriculum included remote training sessions on the PX beamlines at SSRL, and participants collected and analyzed data remotely. Course materials and undergraduate teaching materials were disseminated through the workshop web site, and an open virtual *iLinc* meeting room was made available to all participants for post-workshop collaboration and consultation.

### 6. Concluding remarks

In the context of rapidly evolving educational technologies and the advent of the Web 3.0 decade, this article has high-

lighted some of the innovative and effective implementations in crystallography education and training on the World Wide Web at various points in time. While there is a disproportion in the implementation of contemporary technologies into our global crystallography education resources, the Web 3.0 decade affords ample opportunities to transform education in crystallography. Teaching the science of crystallography has never been more essential. However, we must shift our focus from simply imparting content knowledge to empowering students with the fundamental processes and skills needed for on-demand learning, practice and application in crystallography, skills that can be cultivated quite effectively by cyberinfrastructure. The science of crystallography has always pushed the boundaries of technology. Now is the time to push them again, not just to advance our research capabilities, but to attract and train the next generation. The future is here, and it does not have to be unevenly distributed.

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