not penalized). During training and beyond, I insist on students acting safely using practices that are described in the laboratory manual[11]; I also insist on anyone who enters the laboratory following the same rules.

Further resources on laboratory management, mentoring skills and the funding of undergraduate research can be found on the websites of the Howard Hughes Medical Institute[12], the Council for Undergraduate Research[13] and the American Chemical Society[14]. It is also worth noting that there are opportunities available for undergraduate researchers to be involved in wider community events. For example, competitions exist in synthetic biology[15] and biomolecular design[16] that allow undergraduates to present their projects, and for both students and their mentors to get together and discuss best practices.

One last thing...be kind

If novice students are afraid of your emotional response to mistakes they unwittingly make or misunderstandings they display, they will not be open with you about their work or come to you for guidance. They will also develop negative associations with what should, hopefully, be a joyful experience. As a side effect, the atmosphere among others in the laboratory will also suffer. For every 'macho' student that flourishes in an intimidating, high-pressure environment, many more students will be soured on research and lost to the practice of science. Research leaders are under pressure to produce results for publication, promotion and funding; passing on this pressure to undergraduates does them a disservice, and it is your job to shield them from most of it. I make it clear to students that wanton safety violations, serious breach of promises or dishonest behaviour are the only time they will be sanctioned.

Uri Alon describes a good laboratory as "a nurturing environment that aims to maximize the potential of students as scientists and as human beings", where students are not viewed merely as means to ends of a project[17]. He describes motivated research groups[18] as places where competence, confidence, autonomy and social connectedness coalesce into a gestalt. I endorse this view wholeheartedly. ❐

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References

1. Linko, V. & Dietz, H. *Curr. Opin. Biotechnol.* **24,** 555–561 (2013).
2. Thiry, H. & Laursen, S. L. *J. Sci. Edu. Technol.* **20,** 771–784 (2011).
3. http://seemanlab4.chem.nyu.edu/NedlabTrainingProtocols.htm
4. Kallenbach, N. R., Ma, R. I. & Seeman, N. C. *Nature* **305,** 829–831 (1983).
5. Ma, R. I., Kallenbach, N. R., Sheardy, R. D., Petrillo, M. L. & Seeman, N. C. *Nucleic Acids Res.* **14,** 9745–9753 (1986).
6. Winfree, E., Liu, F. R., Wenzler, L. A. & Seeman, N. C. *Nature* **394,** 539–544 (1998).
7. Zheng, J. P. *et al. Nature* **461,** 74–77 (2009).
8. He, Y., Chen, Y., Liu, H. P., Ribbe, A. E. & Mao, C. D. *J. Am. Chem. Soc.* **127,** 12202–12203 (2005).
9. http://www.afmhelp.com
10. Seeman, N. C. *Sci. Am.* **290,** 64–75 (2004).
11. http://lukemanlab.org/contactus.html
12. http://www.hhmi.org/educational-materials/lab-management/for-early-career-scientists
13. http://www.cur.org/publications/how_to_series/#STEM
14. http://www.acs.org/content/acs/en/education/students/college/research.html
15. http://biomod.net
16. http://igem.org
17. Alon, U. *Mol. Cell* **35,** 726–728 (2009).
18. Alon, U. *Mol. Cell* **37,** 151–152 (2010).

Learning and research in the cloud

Krishna Madhavan, Michael Zentner and Gerhard Klimeck

Research and teaching in nanoscience can, and should, be thought as one joint endeavour. nanoHUB, a cyberinfrastructure that aims to use interactive cloud-based software to meet the needs of both code developers and end-users, is redefining research and education in nanoscience and engineering.

Physics Nobel Laureate Carl Wieman has repeatedly called for physics teachers to use "tools of physics"[1] to teach students scientific concepts. Inherent in this call is the need to tie pedagogical approaches to cutting-edge scientific endeavours and best practices in research. The approach to education therefore needs to evolve as a given field evolves. Fundamental, sometimes revolutionary, changes in a research domain field should be promptly reflected in teaching curricula.

The advent of informatics tools and the Internet has had a profound effect on science and its culture of research and learning. Bainbridge and Roco[2] use the expression "progressive convergence" to describe the disruptive merging of information technology, nanotechnology, biotechnology and cognitive science. In particular, the nanotechnology and information technology components are foundational to this transformation. Nanotechnology provides learners with the opportunity to explore science at the most fundamental scale of nature. Information technology provides the ability to make complex scientific phenomena that are difficult to grasp or visualize more approachable. Because advances in nanotechnology are fuelled by our ability to model and simulate ever-increasing complexity, when coupled together, these two technologies can have a transformative impact on teaching practices and learning strategies in engineering and science.

As the acquisition of new knowledge and the development of characterization and modelling tools progresses at an ever faster pace, the scientific community faces the complex task of disseminating

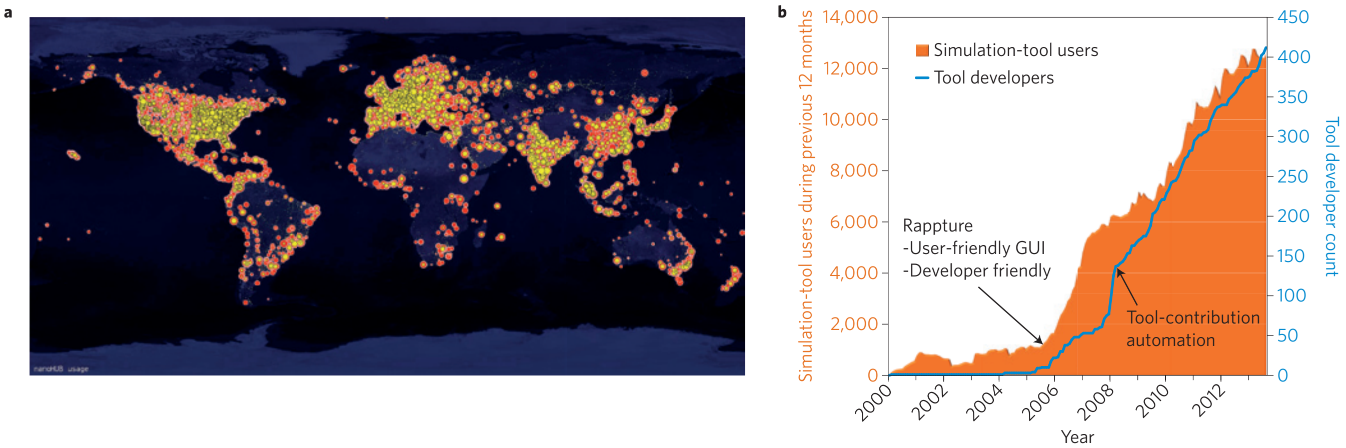

Figure 1 | nanoHUB usage. **a**, World map of nanoHUB usage in 2012. Red symbols indicate user location and their size the number of users from that specific location. Yellow symbols indicate the same data but for simulation-tool users. **b**, Annual number of simulation-tool users (left scale and orange data). Blue line and right scale show the total number of tool developers. Annual number of users and developers increased dramatically after the introduction of user- and developer-friendly GUIs (Rappture). Web-based automation of the tool-contribution process increased the number of tool developers and led to a new growth trend.

scientific results into related research communities and translating new concepts into the educational realm. Coupling nanotechnology and information technology immediately leads to several important scientific, technical and sociological challenges, a number of which are specific to learning. These include finding the most effective way to share research results, modelling and simulation tools with other researchers, educators and students; designing tools that can be useful in both research and learning; finding ways to measure impact; adopting research tools in education faster than conventional knowledge dissemination methods; and creating an educational framework that supports the use of new tools. nanoHUB (www.nanoHUB.org; ref. 3), an online scientific portal related to modelling and simulation, was founded to provide solutions to these challenges.

Sharing results

nanoHUB is a cyberenvironment developed and operated by the Network for Computational Nanotechnology at Purdue University and is funded as a part of the National Nanotechnology Initiative. nanoHUB currently serves over 280,000 users annually distributed over 172 countries (Fig. 1a), which makes it arguably the largest nanotechnology user facility in the world. In the past 12 months, over 13,000 users have run close to 450,000 web-based simulations. More than 400 developers have worked collaboratively on over 350 simulation tools, creating about 1,500 versions of them. Tool revisions reflect both user feedback and, importantly, the continual advancement in research. Each version is registered with a digital object identifier (DOI) that helps in following the evolution of the tool and the research efforts behind it. Furthermore, a DOI allows users to cite a specific version of a specific tool in the scientific literature, enabling scientific data replication by anyone. Over 1,000 papers cite nanoHUB in the scientific literature resulting in an h-index of 51 as of October 2013.

When it was launched in 1998, nanoHUB could run sophisticated UNIX-based science codes through a web-portal[4]. In the first few years, the system was serving a steady number of about 1,000 users per year. It became clear, however, that although web forms are relatively easy to use in 'one-shot' simulations, they do not lend themselves to user-friendly day-to-day research and educational activities. Typically, users need to run multiple simulations and want to compare the results rapidly in an interactive data management and visualization system without repeated, tedious data downloads. In 2005, when interactive graphical user interfaces (GUIs) based on a toolkit called Rappture[5] were introduced, the number of users sharply increased (Fig. 1b).

Usage data from nanoHUB indicates that users are significantly more likely to use the tools in an environment with a rich, interactive graphical interface. Interactivity is an important aspect of the growth of nanoHUB, because it speeds up the answer to 'What if…' queries of learners by giving immediate feedback. Students are invited to try out different options and variables though the GUI, rather than being penalized with tedious intermediate tasks before they can find out the answer. For example, students can seamlessly explore the changes in the optical absorption spectrum of pyramidal quantum dots, as well as appreciate the symmetries of the various eigenstates, as they vary the geometrical parameters of the system[6,7]. In this way, complex software that is usually used in research is accessible in a classroom-friendly interface.

On the other hand, simulation-tool developers may have neither the incentive nor the training to create advanced GUIs and data management systems for an interactive web-based platform. To this end, unlike most portals that require dramatic changes to the science codes for tools to be housed 'on the web', nanoHUB requires no changes to the scientific code base. Once tools have been incorporated into nanoHUB, Rappture allows the developers to test, debug and expand their own tools usually more rapidly than they would be able to do in normal research platforms, which sometimes lack a GUI altogether. The number of developers began to grow rapidly with the introduction of Rappture and grew even further when the formal contribution process was streamlined (Fig. 1b).

nanoHUB is as an efficient, 24/7 stable platform to share information between researchers, educators and students. It supports the needs of very different stakeholders: end-users and science code developers. Developers remain continually engaged, upgrading and innovating the platform as new knowledge is acquired, while end-users have access to authentic research codes with user-friendly GUIs.

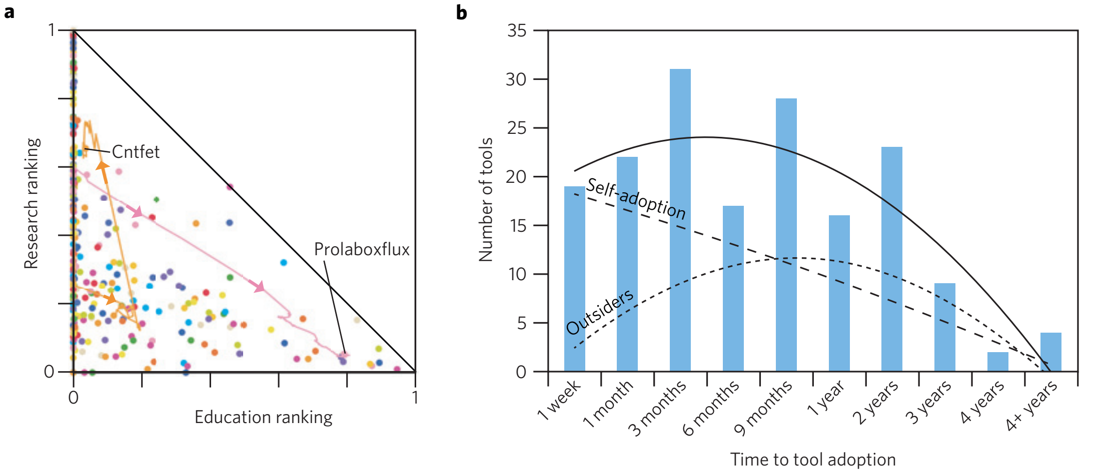

Figure 2 | Tool classification and adoption analytics. **a**, Each simulation tool is represented as a dot as a function of educational and research ranking. Horizontal ranking indicates intensity of use in education. Vertical axis indicates intensity of use in research. Tools may be introduced by a researcher and then adopted in a classroom or vice versa. The time evolution of two tools are indicated through time development trajectories (pink and orange). **b**, Histogram of adoption time of simulation tools in formalized classroom settings. Lines are guides to the eye for tools that are adopted for education on the same campus where the tool is created (self-adoption) and by outside organizations. Median adoption time is less than 6 months.

Using information and tool classification

The presence of more than 13,000 simulation-tool users annually on a nationally funded resource naturally begs the questions: What are these users doing? Is nanoHUB supporting research or education or both?

Our internal data of correlated simulation-tool usage patterns show that nanoHUB is being widely used in systemic, formal learning settings. As of June 2013, nanoHUB had been used as a teaching tool in over 1,000 academic courses, benefiting almost 20,000 students across the globe. It is particularly encouraging to see that the research output available in nanoHUB is actively used in a teaching environment, when in academia, and particularly in engineering and science at the undergraduate level, research and education are sometimes seen as mutually exclusive endeavours[8].

Each simulation tool in nanoHUB is classified through two independent ranking models that quantify usage in either research or education. Some of these data are reported in Fig. 2a. The tools that lie on the abscissa mean that they have been exclusively used in education, those in the ordinate in research. Almost half of the tools lie in the *xy*-plane, indicating that they have been used in education as well as in research, with a substantial percentage of them sitting midway from both axes. Moreover, whether the tool is used mainly for research or education evolves over time. There are examples of tools that were originally designed with educational purposes in mind that migrated towards research, although it is more typical that research tools find adoption in educational settings after sometime (Fig. 2a).

Figure 2b shows that the median time between the publication of a tool and its first adoption in a classroom is less than 6 months. Particularly encouraging is the fact that the median of outside adoption — that is, adoption by faculty members who were not involved in the development of the tool — peaks at 9 months. This adoption rate of new, research-level material is notably faster compared with the typical writing time of a scientific textbook (about 4 years).

Collectively these data show that tools that originated for research purposes can be used with relative ease in formal education, that there is scope for dual use of these tools, and that new research can diffuse rapidly into the classroom.

Early identification of learning contexts

The educational philosophy behind nanoHUB is heavily informed by the *How People Learn* framework[9], which sets guidelines to leverage collective expertise and establish large communities that focus on learning. nanoHUB provides a platform where the scientific community can get together, share their expertise and bring in best practices in research for the benefit of learners. Furthermore, nanoHUB has developed tools to assess how these large communities form and to understand their dynamics. Our user-flow analytics can help identify potential learning contexts in which nanoHUB can play a proactive role[10]. One example is the use of nanoHUB for model eliciting activities[11] — open-ended mathematical modelling problems that require the development of generalizable (shareable, reusable and modifiable) solutions with the intent to teach students problem-solving skills necessary for designing effective modelling and simulation tools.

In the near future, nanoHUB will embrace the 'big data' paradigm to personalize learning and research, along the lines of the US National Academy of Engineering's grand challenge on personalizing learning[12]. Using automated analytics, we will be able to identify the habits and needs of individual learners, group and categorize similar behaviours and connect different users and content for research collaborations, classroom learning, or self-study.

nanoHUB also already contains over 90 complete classes in nanoscience and nanotechnology. However, we resist the temptation to call it a massive open online course (MOOC), even though it is massive, open, online and offers courses. This is principally because nanoHUB has the dual mission of enabling learning and research at the same time, whereas MOOCs only focus on learning. Furthermore the nanoHUB courses have been completely open without formalized subscription and testing of student learning outcomes. These are significant distinctions. Recently we have begun to explore a differently structured online educational approach called nanoHUB-U that transcends classical disciplines as it is geared towards anyone with a bachelor degree in any science or engineering area. Short 20-minute lectures delivered in 5-week modules are coupled with hands-on simulation exercises and integrated testing and certification.

Conclusions

There is significant research that shows that engineering and science are best learned through tactile, hands-on experiences[13]. There have also been major national reports[14] that call for a 'platform perspective' to cyberlearning, and cloud-like environments can provide exactly this. In nanoscience and engineering, where models and simulations play a significant role, nanoHUB offers an easily accessible learning infrastructure that connects teachers and students with the research community. Such cyberenvironments can act as a translational agent that helps transfer new knowledge and methods to learners and researchers in ways that were not possible before. ❐

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References

1. Wieman, C. E. & Perkins, K. K. *Phys. Today* **58,** 36–41 (November, 2005).
2. Bainbridge, W. S. & Roco, M. C. (eds) in *Managing Nano-Bio-Info-Cogno Innovations: Converging Technologies in Society* Ch. 1, 1–7 (Springer, 2006).
3. Klimeck, G., McLennan, M., Brophy, S. B., Adams, G. B. III & Lundstrom, M. S. *Computing Sci. Eng.* **10,** 17–23 (2008).
4. Kapadia, N. H., Fortes, J. B. & Lundstrom, M. S. *ACM Trans. Model. Computer Simulations* **10,** 39–57 (2000).
5. McLennan, M. & Kennell, R. *Computing Sci. Eng.* **12,** 48–53 (2010).
6. Klimeck, G. *et al.* Quantum Dot Lab (2011); https://nanohub.org/resources/qdot
7. Steiger, S., Povolotskyi, M., Park, H-H., Kubis, T. & Klimeck, G. *IEEE Trans. Nanotechnol.* **10,** 1464–1474 (November, 2011); http://dx.doi.org/10.1109/TNANO.2011.2166164
8. Boyer Commission on Educating Undergraduates in the Research University *Reinventing Undergraduate Education: A Blueprint for America's Research Universities* (1998); http://www.niu.edu/engagedlearning/research/pdfs/Boyer_Report.pdf
9. Bransford, J. D., Brown, A. L. & Cocking, R. R. *How People Learn* (National Academy Press, 2000).
10. Mehrotra, S., Zentner, L., Klimeck, G. & Vasileska, D. *IEEE Nanotechnol. Conf.* 932–936 (2011); http://dx.doi.org/10.1109/NANO.2011.6144581
11. Diefes-Dux, H. A., Hjalmarson, M. A. & Zawojewski, J. S. *J. Eng. Edu.* **102,** 179–216 (2013).
12. National Academy of Engineering *Grand Challenges for Engineering in the 21st Century* (2008); http://www.engineeringchallenges.org/
13. Millard, D. L., Chouikha, M. & Berry, F. in *Annu. Conf. Am. Soc. Eng. Edu.* AC2007-1222 (2007); http://go.nature.com/2NTtgz
14. Borgman, C. L. *et al. Fostering Learning in a Networked World: The Cyberlearning Opportunity and Challenge* (National Science Foundation, 2008); http://www.nsf.gov/pubs/2008/nsf08204/nsf08204.pdf

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nanoHUB spans a 15-year effort and involves contributions from over 1,000 people. As such it is impossible to list all contributors. We recognize and acknowledge: M. S. Lundstrom the creator of nanoHUB, M. McLennan who created Rappture and directs the HUBzero effort, R. Kennell who created the middleware that currently powers all nanoHUB simulations, and finally S. Datta who embraced nanoHUB for the development of all his fascinating quantum transport classes over the past 10 years. This work was supported with funding from NSF grants EEC-0228390, EEC-0634750, OCI-0438246, OCI-0721680, EEC-0956819, and EEC-1227110. The visionary leadership of L. Preston and M. Roco is also gratefully acknowledged.

An education in progress

Tebello Nyokong and Janice Limson

In recent years, South Africa has, like other countries, increased investment in nanotechnology research, which in turn has had an effect on the curricula of its higher-education institutions. However, the focus of these changes, and the approach taken to achieve them, are unique to the circumstances of the country.

In all higher-education institutions, curricula change over time. Courses will evolve to keep abreast of emerging areas and this process can be shaped by a range of factors. These include the availability of skilled academics and research infrastructure for training students, the demand from industry for graduates skilled in specific areas, and funding opportunities created by national policy. The process can also be influenced by a broader public understanding or appreciation of a field, and interest from potential students to study certain disciplines. In the late 1990s, a comprehensive nanoscience and nanotechnology landscape — be it the necessary academics, equipment, funding or policy — was still to emerge in South Africa. Any meaningful progression of nano-related curricula in higher education was therefore limited.

An emerging nanoscience education

By the mid-2000s, nanotechnology had begun to leave a mark in the curricula of higher-education institutions in South Africa. This development was most likely driven by the increase in research activities in the field at most of the country's universities and science councils. The pace at which the research sector has grown has been determined by funding for both pure and applied research, human resource development, and, crucially, the necessary infrastructure to equip its scientists and students.

Driving much of the funding for nanotechnology research in South Africa has been its National Nanotechnology Strategy[1], which aims to keep pace with international trends and growth in the sector, and is led by the country's Department of Science and Technology. This strategy was drafted in 2003 by a community of researchers and scientists from several institutions who are represented by the South African Nanotechnology initiative (SANi)[2]. SANi, along with industry and science councils, helped to steer a path for many of the major initiatives that shape the current nanotechnology landscape both broadly in South Africa and more specifically in its higher-education institutions.

Published in 2005, the National Nanotechnology Strategy's four point implementation plan sought to develop characterization centres housing state-of-the-art equipment; foster research and innovation networks across traditional disciplines; evolve a clear capacity building programme; and establish flagship programmes to demonstrate the value of nanoscience and nanotechnology. Its