RTFM! Scientific modeling and the generification of software

Long Abstract (with references)

Taking computational chemistry as an example, the aim of the present study is to emphasize the pivotal role of software, and above all, software distribution, on the epistemological status of modeling in computational sciences.

Computational chemistry (which could be defined as the use of computer resources to solve problems in chemistry) is a scientific discipline that emerged at the same time that computers became available in research laboratories[1], and developed with the graphics terminal[2], in the 70s and 80s. When computers became personal, ie a device in the research lab accessible to non specialists, an upheaval appeared in the scientific community: the scientists who were designing the molecular modeling software (the developers) were not any more the same people than those who performed the calculations (the users). Thus, in the 80s and 90s, the problem of the distribution of the software arose, and tensions appeared in the community. Should the software be shared freely? Should it be sold? Should the code source be open? Could (and should) academic institutions benefit from a "technology transfer"? Depending on what kind of licensing?

The computational chemistry community was also involved with two major industries: the computer manufacturers and the pharmaceutical industry, the latter becoming a potential market for the former through modeling software[3]. In a context of changing times (of science fundings, of market opportunities, of academic technology transfers), computational chemistry software turned from user oriented software to market oriented software.

To account for the strategies, tensions, and changes over time in the community, this work explores The Computational Chemistry List (CCL), a mailing list created in 1991 to provide a discussion board to the fledgling community[4]. For twenty years, it has been used as an opinions forum and a platform for

1 John D. Bolcer and Robert B. Hermann, ‘The Development of Computational Chemistry in the United States’, in *Reviews in Computational Chemistry*, ed. by Kenny B. Lipkowitz and Donald B. Boyd (John Wiley & Sons, Inc., 1994), v, 1–63 <http://onlinelibrary.wiley.com/doi/10.1002/9780470125823.ch1/summary> [accessed 14 July 2012].

2 Eric Francoeur, ‘Cyrus Levinthal, the Kluge and the Origins of Interactive Molecular Graphics’, *Endeavour*, 26 (2002), 127–131 <doi:10.1016/S0160-9327(02)01468-0>.

3 Donald B. Boyd, ‘How Computational Chemistry Became Important in the Pharmaceutical Industry’, in *Reviews in Computational Chemistry*, ed. by Kenny B. Lipkowitz and Thomas R. Cundari (John Wiley & Sons, Inc., 2007), XXIII, 401–451 <http://onlinelibrary.wiley.com/doi/10.1002/9780470116449.ch7/summary> [accessed 15 July 2012].

4 Jan K. Labanowski, ‘Free Speech, Quality Control, and Flame Wars’, *Academe*, January 2007 <http://www.aaup.org/AAUP/pubsres/academe/2007/JF/Feat/Lear.htm> [accessed 13 October 2011].

scientific exchange. Since its inception, through the archives of its thousands of threaded conversations, the mailing list is a valuable corpus from a Goffmanian perspective of the presentation of self[5], with its "trolls" and "flame wars" particularly helpful in revealing the tensions and controversies within the community[6].

The main topics of these tensions and controversies were the issue of software and the scientific modeling activity. From an epistemological point of view, an “epochal break”[7] of scientific modeling activities, from a culture of explanation to a culture of prediction[8], has been linked to the availability of the ubiquitous desktop computer, thus empowering computational science practitioners with respect to expert computing scientists, equipped with supercomputing facilities. I hereby argue, following previous work on organizational software[9] that the scientific modeling software concomitantly turned into the process of “generification”[10], unveiling the mutual shaping of the modeling scientific activity and the technological device, thus provoking many tensions in the scientific computational community.

5 D.A. Grier and M. Campbell, ‘A Social History of Bitnet and Listserv, 1985-1991’, *IEEE Annals of the History of Computing*, 22 (2000), 32–41 <doi:10.1109/85.841135>.

6 Gabriella Coleman, ‘Phreakers, Hackers, and Trolls: The Politics of Transgression and Spectacle.’, in *The social media reader*, ed. by Michael Mandiberg (New York: New York University Press, 2012), pp. 99–119 <http://site.ebrary.com/id/10535662> [accessed 5 April 2012].

7 Alfred Nordmann, *Science Transformed? Debating Claims of an Epochal Break* (University of Pittsburgh Pre, 2011).

8 Ann Johnson and Johannes Lenhard, ‘Toward a New Culture of Prediction: Computational Modeling in the Era of Desktop Computing.’, in *Science Transformed?: Debating Claims of an Epochal Break*, ed. by Alfred Nordmann, Hans Radder, and Gregor Schiemann (University of Pittsburgh Pre, 2011), pp. 189–200.

9 Neil Pollock and Robin Williams, *Software and Organisations: The Biography of the Enterprise-Wide System or How SAP Conquered the World*, 1st edn (Routledge, 2008).

10 Neil Pollock, Robin Williams and Luciana D’Adderio, ‘Global Software and Its Provenance: Generification Work in the Production of Organizational Software Packages’, *Social Studies of Science*, 37 (2007), 254–280.