CHARLES BABBAGE INSTITUTE

CENTER FOR THE HISTORY OF INFORMATION TECHNOLOGY

NEWSLETTER
Vol. 39 No. 2
Fall 2017

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Calvin Mooers Papers Connecting Computers and Molecules (Norberg Grant)

Two of the most prominent trends in science, technology, and medicine since World War II are the increasing focus on matter at the *molecular* level (molecular biology, nanotechnology, rational drug design) and the ever-broader use of *computer*-based tools and methods. We usually think of these as separate developments, linked only insofar as each has brought about sweeping transformations eagerly taken up by the other. For example, molecular-level materials science has fueled the advances in computing hardware that power Moore's Law, and computing has enabled the transformation of the lab science of molecular genetics into the information science of genomics. However, my research shows that the molecularization and computerization of recent science, technology, and medicine are even more deeply connected. The molecular sciences and scientific computing share a common foundation in the project of studying molecules and storing information about molecules on computers. My goal is to tell the history of these ways of knowing the material world at the scale of nanometers and terabytes, in a book tentatively entitled *The Molecular World: How Molecules Became Digital, and Everything Became Molecules*.

So far, my research has addressed such topics as the role of molecular databases in shaping environmental regulation in Europe and America, the role of nineteenth-century molecular diagrams in the genesis of the mathematical field of graph theory, and the role of molecular synthesis and structure determination as crucial domains for early work in expert systems artificial intelligence. This research also builds upon a separate book project that I am currently wrapping up, a history of chemistry in the late nineteenth and early twentieth centuries told through the lens of chemical information, entitled *Naming Matters: Nomenclature and the Structure of Modern Chemistry*. Thanks to a Norberg Travel Grant, I was able to gather crucial material for knitting together these stories through a visit to the Charles Babbage Institute.

My focus during this visit was the Calvin N. Mooers Papers (CBI 81). Mooers, a pioneer of American information science, has emerged as a pivotal figure in the story that I would like to tell. Best known as the founder of the field of information retrieval, the erstwhile mathematician and IT entrepreneur played a crucial role in developing data structures suitable for mechanical and electronic handling of information about chemical compounds. During the late 1940s, Mooers helped to lay the foundation for the contemporary field of chemical information, a multi-billion-dollar industry and a crucial part of the infrastructure of the modern life, environmental, and materials sciences. In doing so, he reunited the fields of chemical documentation and graph theory. Both of these subjects had roots in the systematic study of patterns in chemical formulas during the late nineteenth century, but they had developed along parallel tracks until Mooers brought them back together.

Delving into the voluminous personal correspondence, technical notes and reports, and artifacts in the Mooers papers, I discovered a man with a unique gift to be at the right place at the right time with precisely the wrong attitude. During the late 1940s, he was an anti-institutionalist, thumbing his nose at Vannevar Bush even as he pursued a field shaped by Bush's Memex

concept and sought support from MIT personnel fiercely loyal to Bush. During the 1960s and 70s, the heyday of ALGOL and FORTRAN, Mooers fought for strong intellectual property rights for the creators of programming languages. I was also able to consult examples of the original mechanical card-sorting machines that Mooers developed for the fascinating but ill-fated Zator company that he founded. The crucial contributions of Calvin Mooers' wife Charlotte to their research and business enterprises, which he acknowledged but which are difficult to identify in his published work, emerge more clearly within the archives as well.

I encourage readers who would like to learn more to take a look at the fascinating oral history of Calvin and Charlotte Mooers that the Charles Babbage Institute has made available online. I look forward to bringing the research that I conducted at CBI into articles for scholarly audiences and the interested public, as well as into my teaching in both the history of science and technology and in chemical information literacy and cheminformatics. Everyone at the Charles Babbage Institute went out of their way to help me make my visit a success. I thank them for all of their help and encourage others with interest in the history of computing to take advantage of this magnificent resource!

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