
RTFM! Scientific modeling and the generification of software

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Abstract

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 is a scientific discipline that emerged at the same time that computers became available in research laboratories, and developed with the graphics terminal, in the 70s and 80s. When computers became personal, an upheaval appeared in the scientific community: the scientists who were designing the molecular modeling software (the developers) were not any more the same persons 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. In a context of changing times (of science fundings, of market opportunities, of academic technology transfers) and in the middle of two giant industries (computer manufacturers and the Big Pharma), computational chemistry software turned from user oriented software to market oriented software.

Concomitantly to an "epochal break" of scientific modeling activities, from a culture of explanation to a culture of prediction, the scientific modeling software turned into the process of "generification", unveiling the mutual shaping of the modeling scientific activity and the technological device.

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