

# The subtle impacts of software on trust

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Computational reproducibility (i.e. issues of reproducibility stemming from the computer as a scientific tool) possesses its own dynamics and narratives of crisis. Alongside the difficulties of computing as an ubiquitous yet complex scientific activity, computational reproducibility suffers from a naive expectancy of total reproducibility and a moral imperative to embrace the principles of free software as a non-negotiable epistemic virtue.

We argue that the epistemic issues at stake in actual practices of computational reproducibility as an element of trust in computational methods need to focus on software as a pivotal concept, one that is surprisingly often overlooked.

Software is not only about designing and coding but also about maintaining, supporting, distributing, licensing, and governance; it is not only about developers but also about users. We focus on openness debates among computational chemists involved in molecular modeling software packages as empirical grounding for our argument.

We then identify and analyze four epistemic characteristics (transparency, consistency, sustainability and inclusivity) as key to the role of software in establishing trust in computational methods.