PLUMED: A “community” project for enhanced sampling

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The landscape of computational physics, chemistry, and biology is undergoing rapid transformation. Online repository services like GitHub and GitLab have dramatically lowered barriers to code sharing, while generative AI promises to make software development accessible to individual research groups. These technological shifts raise important questions about the future of traditional molecular dynamics software packages, which typically rely on small developer teams serving much larger user communities.

In response to these changes, many software development groups have prioritized reproducibility by creating online repositories for sharing computational results. While these efforts have yielded impressive projects, a critical challenge remains unaddressed: how to encourage broad adoption of these new tools beyond their immediate development communities.

The common discourse around "community-driven" software development presents its own complications. This framing suggests a web of mutual obligations among users that may inadvertently constrain scientific creativity and innovation. However, this does not mean collaborative software development lacks value—rather, it requires more thoughtful approaches to fostering genuine collaboration without imposing restrictive social contracts.

This talk will examine our experiences with PLUMED over recent years, exploring how collaborative software projects can balance openness and accessibility with the creative freedom essential for scientific advancement.