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The KMOS Kinetic Monte Carlo Framework

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Abstract:

KMOS is a versatile, general purpose, extensible kinetic Monte Carlo simulation framework. During these hands-on sessions, participants will get first hand experience on using its most important features. After an introduction to the kmos data model, participants will learn how to analyze, compile and run existing kmos models, as well as to perform analysis of results. Both the graphical user interface (GUI) and the more powerful application programming interface (API) will be covered. Once they are familiarized with these basic concepts, participants will implement their own kMC models from scratch using the API and apply previously learned concepts to them. Finally, some current kMC challenges and the state of kmos development will be discussed.