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Advancing the Computational Molecular Sciences through Better Theory and Better Software

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This lecture will outline the goals of the Molecular Sciences Software Institute and the leading initiatives in software infrastructure, education, and community outreach that the institute engages in. These activities span the domain of the computational molecular sciences, which includes electronic structure theory, bio-/macro-molecular simulation, and computational materials science. We will then transition to some detail of the software architecture of the MolSSI Quantum Chemistry Archive project for computing, sharing, and analyzing quantum chemistry data at scale. These details will highlight the challenges and possible solutions when moving to cloud resources, distribution and containerization of programs, and reproducibility issues while still maintaining interoperability with canonical academic campus and leadership computing facilities.

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