

Development of qmcPACK

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Quantum Monte Carlo (QMC) methods can, in principle, calculate exact properties of many-body systems. With recent developments in QMC algorithms and ever-growing computing powers, QMC methods have become powerful and practical tools to study a wide range of problems with direct connections to high pressure physics, materials science, surface science, the theory of strongly correlated electrons and low-temperature physics.

We are developing comprehensive computational frameworks for QMC simulations built upon the innovative algorithms and numerical methods for the advanced computing environments of today and future. One of the components of the tools is qmcPACK, an object-oriented QMC code. qmcPACK is the computational core of our tools and is the building block for future developments in QMC algorithms and materials simulation tools.