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Intricacies of modern supercomputing illustrated with recent advances in simulations of strongly correlated electron systems

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The continued thousand-fold improvement in sustained application performance per decade on modern supercomputers keeps opening new opportunities for scientific simulations. But supercomputers have become very complex machines, built with thousands or tens of thousands of complex nodes consisting of multiple CPU cores or, most recently, a combination of CPU and GPU processors. Efficient simulations on such high-end computing systems require tailored algorithms that optimally map numerical methods to particular architectures. These intricacies will be illustrated with simulations of strongly correlated electron systems, where the development of quantum cluster methods, Monte Carlo techniques, as well as their optimal implementation by means of algorithms with improved data locality and high arithmetic density have gone hand in hand with evolving computer architectures. The present work would not have been possible without continued access to computing resources at the National Center for Computational Science of Oak Ridge National Laboratory, which is funded by the Facilities Division of the Office of Advanced Scientific Computing Research, and the Swiss National Supercomputing Center (CSCS) that is funded by ETH Zurich.