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Challenges for Large Scale Simulations

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With computational approaches becoming ubiquitous the growing impact of large scale computing on research influences both theoretical and experimental work. I will review a few examples in condensed matter physics and quantum optics, including the impact of computer simulations in the search for supersolidity, thermometry in ultracold quantum gases, and the challenging search for novel phases in strongly correlated electron systems. While only a decade ago such simulations needed the fastest supercomputers, many simulations can now be performed on small workstation clusters or even a laptop: what was previously restricted to a few experts can now potentially be used by many. Only part of the gain in computational capabilities is due to Moore's law and improvement in hardware. Equally impressive is the performance gain due to new algorithms - as I will illustrate using some recently developed algorithms. At the same time modern peta-scale supercomputers offer unprecedented computational power and allow us to tackle new problems and address questions that were impossible to solve numerically only a few years ago. While there is a roadmap for future hardware developments to exascale and beyond, the main challenges are on the algorithmic and software infrastructure side. Among the problems that face the computational physicist are: the development of new algorithms that scale to thousands of cores and beyond, a software infrastructure that lifts code development to a higher level and speeds up the development of new simulation programs for large scale computing machines, tools to analyze the large volume of data obtained from such simulations, and as an emerging field provenance-aware software that aims for reproducibility of the complete computational workflow from model parameters to the final figures. Interdisciplinary collaborations and collective efforts will be required, in contrast to the cottage-industry culture currently present in many areas of computational condensed matter physics.