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## **Multi-Length Scale Matrix Computations and Applications in Quantum Mechanical Simulations**

Multi-length scale matrices refer to a class of matrices where dimensionality, eigenvalue and singular value distributions of the matrices can be characterized by a set of parameters.

In the parameter space of interest, the matrices could be extremely large in dimensionality and ill-conditioned. In this talk, we will first describe a range of our synergistic activities

in recent years on development of robust and efficient linear algebra solvers and high-performance software for multi-length scale matrix computation problems arising from quantum mechanical simulations of materials. We will also discuss the feasibility, through the use of tensor-based computation, of 10000-electron simulations on regular desktop PCs to

allow physicists and chemists addressing important questions concerning properties of materials, such as magnetism and superconductivity.