Development of large-scale time-dependent density functional theory based on massively-parallel sparse-matrix library

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Abstract

The computational prediction for the chemical reactivity and electronic properties in large-scale molecules composed of several thousand to ten thousand atoms, such as supramolecules and biomolecules, plays an important role in drug discovery and nanomaterial design. Therefore, an algorithm is needed to calculate large molecular excited states with high accuracy. Time-dependent density functional theory (TDDFT) is becoming a popular methodology for computing excited states because of its reasonable cost and relatively high accuracy. Nevertheless, this inherent cubic scaling still limits the accessible system sizes to some hundred atoms, and routine TDDFT calculations are usually only done in this regime.

In this work, we have developed a memory-distributed parallel TDDFT program for calculating the response properties of large-scale molecules. In the implementation, each response property is represented by the n-th order density matrix divided and distributed to each computer node. The trial vectors in the iterative Davidson method are also distributed and parallelized. All the matrix multiplications are performed using NTPoly library, which is a massively parallel library for computing the functions of sparse, symmetric matrices.