# parallel quantum dynamics with Smolyak algorithm for general molecular simulation

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## ABSTRACT

A parallelized general quantum dynamics package using Smolyak algorithm is introduced in this work. Taking advantage of the Smolyak sparse grids for high-dimensional problems, the simulation could be performed with high accuracy, and in the meantime, impressive parallel efficiency. Three MPI schemes are implemented to adapt different kinds of machines. The capability of the simulation could be generally up to tens of degrees of freedom for the propagation of hundreds of femtoseconds. It could be further improved to hundreds of degrees with a bath-system separation scheme in the framework of Smolyak method. A few direct applications, compared with other methods, are presented finally as examples and the verification of the code.

### References

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