Summary: In the general field of quantum information and computation, quantum walks are playing an increasingly important role in constructing physical models and quantum algorithms. We have recently developed a distributed memory software package \textit{pyCTQW}, with an object-oriented Python interface, that allows efficient simulation of large multi-particle CTQW (continuous-time quantum walk)-based systems. In this paper, we present an introduction to the Python and Fortran interfaces of \textit{pyCTQW}, discuss various numerical methods of calculating the matrix exponential, and demonstrate the performance behavior of \textit{pyCTQW} on a distributed memory cluster. In particular, the Chebyshev and Krylov-subspace methods for calculating the quantum walk propagation are provided, as well as methods for visualization and data analysis.

MSC:

- 81-04 Software, source code, etc. for problems pertaining to quantum theory
- 81-08 Computational methods for problems pertaining to quantum theory
- 81S25 Quantum stochastic calculus
- 81P45 Quantum information, communication, networks (quantum-theoretic aspects)

Keywords:
continuous-time quantum walk; multiple walkers; Padé approximant; Krylov subspace method; Chebyshev matrix expansion

Software:
F2PY; MATLAB \texttt{expm}; pyCTQW; PETSc; Expokit; SLEPc

Full Text: DOI

References:


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