

# Quantum Trajectories with Dynamic Loop Scheduling and Reinforcement Learning

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## Abstract

The quantum trajectory method (QTM) is one approach in simulating wave packet dynamics. Based on the hydrodynamic formulation of quantum mechanics, the QTM represents a wave packet by an unstructured set of pseudo-particles whose trajectories are coupled by the quantum potential. The solution of the governing equations involves three computationally-intensive parallel loops, each loop having nonuniform iterate execution times, justifying the use of dynamic loop scheduling. However, specifying a single scheduling technique for the three loops for the whole duration of the simulation may not achieve the highest possible performance since the loops have different characteristics, and that these characteristics vary as the simulation progresses.

The contribution of this paper is a strategy based on reinforcement learning (RL) for improving the performance of wave packet simulations, as well as other time-stepping scientific applications with computationally-intensive parallel loops. The strategy employs a RL agent following a model-free learning approach, to select the most appropriate scheduling technique for a parallel loop, while the simulation is in progress.

Preliminary timing tests indicate that the parallel cost of the simulation with the RL

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agent is up to 45% less than the lowest cost of the simulation with a fixed scheduling technique.

Keywords: quantum trajectories, dynamic loop scheduling, reinforcement learning

## 1 Introduction

Time-dependent wave packets are widely used to model various phenomena in physics. Classical approaches for computing the wave packet dynamics include space-time grids, basis sets, or combinations of these methods. An unstructured grid approach, the quantum trajectory method (QTM), based on the hydrodynamic interpretation of quantum mechanics by Bohm [7], was implemented for a serial computing environment by Lopreore and Wyatt [22]. The QTM solves the quantum hydrodynamic equations using a moving weighted least-squares (MWLS) algorithm to compute needed derivatives. The solutions to the equations of motion give the quantum trajectories for “fluid particles” or pseudoparticles.

A simulation code for wave packet dynamics using the QTM on a shared-memory environment was developed by Brook *et al.* [8]. Starting from a serial code that utilizes an implicit update scheme, OpenMP parallelizing directives were inserted before computationally-intensive loops. Message-passing versions of the simulation code, using MPI for communications, were developed by Cariño *et al.* integrating dynamic loop scheduling [13], adaptivity in the MWLS algorithm [14, 15], and an alternate wave packet initialization scheme [36].

A problem associated with the use of dynamic loop scheduling is the selection of the loop scheduling technique that will obtain the highest possible performance. This problem is not unique to wave packet simulations; it generally occurs in any scientific application that involves a computationally intensive parallel loop with nonuniform iterate execution times. The selection problem becomes complicated when there are several such loops in a single application, each loop potentially requiring a different scheduling technique for