Software paper for submission to the Journal of Open Research Software

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(1) Overview

Title

spinsim: a GPU optimised solver of spin one and half quantum systems

The title of the software paper should focus on the software, e.g. "Text mining software from the X project". If the software is closely linked to a specific research paper, then "Software from Paper Title" is appropriate. The title should be factual, relating to the functionality of the software and the area it relates to rather than making claims about the software, e.g. "Easy-to-use".

Paper Authors

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Original conception of released version of algorithm.

1. First author role and affiliation
2. Second author role and affiliation etc.

Abstract
A short (ca. 100 word) summary of the software being described: what problem the software addresses, how it was implemented and architected, where it is stored, and its reuse potential.

Keywords
Time dependent Schrödinger equation; Spin one; Spin half; Integrator; GPU;

keyword 1; keyword 2; etc.
Keywords should make it easy to identify who and what the software will be useful for.

Introduction

Motivation

Spinsim is a package for python designed to simulate the spin one dynamics of Bose Einstein Condensates, specifically for the Spinor BEC lab group at Monash University.

Motivation

An overview of the software, how it was produced, and the research for which it has been used, including references to relevant research articles. A short comparison with software which implements similar functionality should be included in this section.

Implementation and architecture
How the software was implemented, with details of the architecture where relevant. Use of relevant diagrams is appropriate. Please also describe any variants and associated implementation differences.

Quality control
Detail the level of testing that has been carried out on the code (e.g. unit, functional, load etc.), and in which environments. If not already included in the software documentation, provide details of how a user could quickly understand if the software is working (e.g. providing examples of running the software with sample input and output data).

(2) Availability

Operating system
Tested on Windows 10
Please include minimum version compatibility.

Programming language
Python (3.7 or greater)
Please include minimum version compatibility.

Additional system requirements
Nvidia cuda compatible GPU.
E.g. memory, disk space, processor, input devices, output devices.

Dependencies
numba (0.50.1 or greater)
numpy (1.19.3)
matplotlib (for example code, 3.2)
neuralsense (for benchmark code)
E.g. libraries, frameworks, incl. minimum version compatibility.

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Original conception of released version of algorithm.
Please list anyone who helped to create the software (who may also not be an author of this paper), including their roles and affiliations.

Software location:
Archive

Name: Monash Bridges
Persistent identifier: e.g. DOI, handle, PURL, etc.
Licence: BSD 3 Clause
Publisher: Alex Tritt

Version published: 1.0.0
Date published: dd/mm/yy

Code repository

Name: GitHub
Persistent identifier: https://github.com/alexander-tritt-monash/spinsim
Licence: BSD 3 Clause
Date published: 18/11/20

Language
English.

Software location:
Archive (e.g. institutional repository, general repository) (required – please see instructions on journal website for depositing archive copy of software in a suitable repository)

Name: The name of the archive.
Persistent identifier: e.g. DOI, handle, PURL, etc.
Licence: Open license under which the software is licensed.
Publisher: Name of the person who deposited the software.
Version published: The version number of the software archived.
Date published: dd/mm/yy

Code repository (e.g. SourceForge, GitHub etc.) (required)

Name: The name of the archive.
Persistent identifier: e.g. DOI, handle, PURL, etc.
Licence: Open license under which the software is licensed.
Date published: dd/mm/yy

Emulation environment (if appropriate)

Name: The name of the archive.
Persistent identifier: e.g. DOI, handle, PURL, etc.
Licence: Open license under which the software is licensed.
Date published: dd/mm/yy

Language
Language of repository, software and supporting files.

(3) Reuse potential
Please describe in as much detail as possible the ways in which the software could be reused by other researchers both within and outside of your field. This should include the use cases for the software, and also details of how the software might be modified or extended (including how contributors should contact you) if appropriate. Also you must include details of what support mechanisms are in place for this software (even if there is no support).

Acknowledgements
Please add any relevant acknowledgements to anyone else who supported the project in which the software was created, but did not work directly on the software itself.

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If the software resulted from funded research please give the funder and grant number.

Competing interests
The authors declare that they have no competing interests.
If any of the authors have any competing interests then these must be declared. The authors' initials should be used to denote differing competing interests. For example: "BH has minority shares in [company name], which part funded the research grant for this project. All other authors have no competing interests."
If there are no competing interests, please add the statement: "The authors declare that they have no competing interests."

References
Please enter references in the Harvard style and include a DOI where available, citing them in the text with a number in square brackets, e.g.

[1] Piwowar, H A 2011 Who Shares? Who Doesn't? Factors Associated with Openly Archiving Raw Research Data. PLoS ONE 6(7): e18657. DOI: http://dx.doi.org/10.1371/journal.pone.0018657.
