

Software paper for submission to the Journal of Open Research Software

To complete this template, please replace the blue text with your own. The paper has three main sections: (1) Overview; (2) Availability; (3) Reuse potential.

Please submit the completed paper to: editor.jors@ubiquitypress.com

(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

1. Tritt, Alexander;
2. Turner, Lincoln David;
3. Saunderson, James;
4. Morris, Joshua;
5. Hochstetter, Joel;

1. Last name, first name; (Lead/corresponding author first)
2. Last name, first name; etc.

Paper Author Roles and Affiliations

1. PhD student, School of physics and astronomy, Monash University
2. Supervisor, School of physics and astronomy, Monash University
3. Supervisor, Department of electrical and computer systems engineering, Monash University
4. Original writer of AtomicPy for spin half systems
5. Original writer of the spin one extension to AtomicPy

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

Please include minimum version compatibility.

Programming language

Please include minimum version compatibility.

Additional system requirements

E.g. memory, disk space, processor, input devices, output devices.

Dependencies

E.g. libraries, frameworks, incl. minimum version compatibility.

List of contributors

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 (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.

Funding statement

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

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>.

Copyright Notice

Authors who publish with this journal agree to the following terms:

Authors retain copyright and grant the journal right of first publication with the work simultaneously licensed under a Creative Commons Attribution License that allows others to share the work with an acknowledgement of the work's authorship and initial publication in this journal.

Authors are able to enter into separate, additional contractual arrangements for the non-exclusive distribution of the journal's published version of the work (e.g., post it to an institutional repository or publish it in a book), with an acknowledgement of its initial publication in this journal.

By submitting this paper you agree to the terms of this Copyright Notice, which will apply to this submission if and when it is published by this journal.