Sustainability of research software, declaration of intention

Algorithms for Lattice Fermions

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Background: the prototype ALF-05

Material science is a complex multi-scale problem such that complementary methods have to be used to describe physics at different energy scale. Low energy collective and emergent phenomena such as superconductivity, topological phases of matter or magnetism, are described by models of interacting fermions on a lattice. The aim of the ALF-package is to provide a unified framework to tackle a number of fermion models within the so called auxiliary field quantum Monte Carlo approach (see Ref. [1] for a review). It provides standards so as to specify very general models, standards to define the lattice structure, and standards to compute different types of observables. Being a stochastic approach, it also comes with an error analysis library. The motivation for such a project is to secure our knowhow in a structured, robust and well documented program package. This allows new generations of PhD students and Postdoctoral researchers to profit from past algorithmic development and optimization so as to efficiently investigate new directions. It also allows to reproduce published results and to play with new ideas within minutes.

Our project is at the prototype level. Our code is to be found on our Git server `http://alf.physik.uni-wuerzburg.de/` which is presently only accessible upon invitation since we are still at a testing level. We have adopted Git since it allows for open communication within the user pool, tracks issues and documents them. Furthermore the history of the code development is stored in the Git such that older versions of the code can be tested against newer ones. At every commit our Git server carries out a set of tests so as to automatically scan for errors. Clearly, such a development framework has become a prerequisite for sustainable code development. ALF-05 has already been used to generate publication quality results. In particular Ref. [2] is one of the first applications of the package.

Quantum Monte Carlo methods are computationally very demanding. One central aspect of the project is to maintain efficiency for general models. Our code heavily relies on BLAS, and comes with a parallel MPI-based implementation. We are in contact with KONWIHR (Kompetenznetzwerk für Wissenschaftliches Höchstleistungsrechnen in Bayern) and with the JSC (Jülich Supercomputing Centre) so as to optimize further the code and to bring it to ever higher programming standards.

User pool
The ALF project is unique. To the best of our knowledge there is no package as general as ours for lattice fermions. The potential pool of users are solid state physicists interested in low temperature collective phenomena. Researchers in the domain of cold atoms *build* models that can be simulated with the ALF-package. We hence foresee that the ALF-package, if easy to use, will find interest in this community so as to benchmark their experimental results. Finally the high energy lattice gauge researchers work with very similar algorithms and models such that we can equally foresee a substantial overlap with this community. To date, our user pool counts researchers at the following institutions: IOP (Institute of Physics) in Beijing, Beijing Normal University, University of California at San-Diego, University of Iowa, RWTH Aachen, University of Erlangen, Jülich Supercomputing Centre and of course the University of Würzburg. As mentioned above, we are still testing the software. Once we believe that it is as user friendly as possible it will be available as an open-source package.

Licence
We have opted to licence the code under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or any later version. The documentation (which we have included here) is licensed under a Creative Commons Attribution-ShareAlike 4.0 International License. This choice of licenses allows for free distribution of the source code.

Goals
The success of such a project relies on dedicated man-power. One has to continually develop and maintain the package, provide user support, communicate with the user pool so as to identify future developments and issues. Our long term goals are to enhance our toolbox of algorithms and to make sure that the package is user friendly. This will allow non-specialists in quantum Monte Carlo methods to use it and literally play with model systems of correlated fermions. We will equally enhance the pool of predefined models, and provide an ever growing set of test cases and reference material.

Requested funding
As it stands this project has essentially been carried out in our *free time* albeit with the help of Dr. F. Goth who is funded by the SFB1170 in the aim of providing support for program development and optimization. To pursue our effort and to achieve our goals we will have to create a small team around our program package. We thus would like to apply for two positions, one senior and one junior, or in other words

One Postdoctoral researcher for 3 years and
One PhD student for 3 years.

Their responsibilities will include the following.

- Ensure that research developments in our field trickle down into our software package

- Ensure that our software runs optimally on novel hardware architectures
- Enhance the scope of the package by include new algorithms and updating schemes
- Provide support for the user pool

To provide training for the program package, we also plan to organize an international workshop. For this we will need a total of 25 K€.

To facilitate development of the package and communication within the user pool we need a robust central infrastructure. We have opted to host our own Gitlab instance and the server will have to be updated to keep up with the demands of the users. With the use of Gitlab we gain version control, effective issue tracking and basic tools for monitoring the workflow. To keep the quality of our software at a high level and to keep the turnaround time for debugging at a minimal level, we employ automated tests and profiling. These tests run on additional, separate machines that will have to be maintained. In addition we foresee the need for virtualized environments so as to have the ability to quickly test our software in different environments. Use cases include the software environments of our users as well as those available at supercomputer centers. To be able to continually provide those high level services we foresee hardware costs of 10 K €.

References

[1] F. Assaad and H. Evertz, in *Computational Many-Particle Physics*, Vol. 739 of *Lecture Notes in Physics*, edited by H. Fehske, R. Schneider, and A. Weiße (Springer, Berlin Heidelberg, 2008), pp. 277–356.

[2] F. F. Assaad and T. Grover, Phys. Rev. X **6**, 041049 (2016).