

The ALPS project release 1.3: open source software for strongly correlated systems

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Abstract

We present release 1.3 of the ALPS (Algorithms and Libraries for Physics Simulations) project, an international open source software project to develop libraries and application programs for the simulation of strongly correlated quantum lattice models such as quantum magnets, lattice bosons, and strongly correlated fermion systems. Development is centered on common XML and binary data formats, on libraries to simplify and speed up code development, and on full-featured simulation programs. The programs enable non-experts to start carrying out numerical simulations by providing basic implementations of the important algorithms for quantum lattice models: classical and quantum Monte Carlo (QMC) using non-local updates, extended ensemble simulations, exact and full diagonalization (ED), as well as the density matrix renormalization group (DMRG). Changes in the new release include a DMRG program for interacting models, support for translation symmetries in the diagonalization programs, the ability to define custom measurement operators, and support for inhomogeneous systems, such as lattice models with traps. The software is available from our web server at <http://alps.comp-phys.org/>.

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1. Introduction

In this paper we present release 1.3 of the ALPS project (Algorithms and Libraries for Physics Simulations), an open source software development project for strongly correlated lattice models. We will present a short overview and focus on new features compared to the previous releases [1, 2].

Quantum fluctuations and competing interactions in quantum many body systems lead to unusual and exciting properties of strongly correlated materials such as quantum magnetism [3], high temperature superconductivity [4], heavy fermion behavior [5], and topological quantum order [6]. The same strong interactions make accurate analytical treatments hard and direct numerical simulations are essential to increase our understanding of the unusual properties of these systems.

The last decade has seen tremendous progress in the development of algorithms. Speedups of many orders of magnitude have been achieved [7–12]. These advances come at the cost of substantially increased algorithmic complexity and challenge the current model of program development in this research field. In contrast to other research areas, in which large “community codes” are being used, the field of strongly correlated systems has so far been based mostly on single codes developed by individual researchers for particular projects. While the simple algorithms used a decade ago could be easily programmed by a beginning graduate student in a matter of weeks, it now takes substantially longer to master and implement the new algorithms. Thus, their use has increasingly become restricted to a small number of experts.

The ALPS project aims to overcome the problems posed by the growing complexity of algorithms and the specialization of researchers onto single algorithms through an open-source software development initiative. In release 1.3 new features desired by ALPS users, especially experimentalists, have been added, as well as a DMRG program for interacting problems.

To quote from the previous publication [1], the goals of the ALPS project are to provide:

- **standardized file formats** to simplify exchange, distribution and archiving of simulation results and to achieve interoperability between codes.
- **generic and optimized libraries** for common aspects of simulations of quantum and classical lattice models, to simplify code development.
- a set of **applications** covering the major algorithms.
- **license** conditions that encourage researchers to contribute to the ALPS project by gaining scientific credit for use of their work.
- **outreach** through a web page [2], mailing lists and workshops to distribute the results and to educate re-

searchers both about the algorithms and the use of the applications.

- **improved reproducibility** of numerical results by publishing source codes used to obtain published results.
- an **archive** for simulation results.

The ready-to-use applications are useful both for *theoreticians* who want to test theoretical ideas about quantum lattice models and to explore their properties, as well as for *experimentalists* trying to fit experimental data to theoretical models to obtain information about the microscopic properties of materials.

In the following, we present a quick review of these aspects of the ALPS project, focusing on new features in release 1.3.

2. File formats

The most basic part of the ALPS project is the definition of common standardized file formats suitable for a wide range of applications. Standardized file formats enable the exchange of data between applications, allow the development of common evaluation tools, simplify the application of more than one algorithm to a given model, and are a prerequisite for the storage of simulation data in a common archive. The ISO standard XML [13] was chosen for the specification of these formats because it has become the main text-based data format on the internet and because it is supported by a large and growing number of tools.

We have designed a number of XML schemas [14] to describe

- the input of simulation parameters,
- the lattices,
- quantum lattice models,
- and the output of results.

A detailed specification of the formats is given on our web pages [2, 14]. As examples we show a lattice and a model definition in figures 1 and 2. Any of the ALPS applications can be run by providing an input file, specifying the simulation parameters, together with lattice and model definitions (figures 1 and 2) to that application (provided the application supports that type of model). Standardized formats that extend across all applications reduce the learning curve for using the applications and allow common tools to be used to analyze the data.

2.1. New features

2.1.1. Lattice definitions

New features in the lattice definitions in release 1.3 include the possibility to specify inhomogeneity and depletion. While in a regular lattice, the model Hamiltonian is the same for all bonds or sites with the same type, in an inhomogeneous lattice the couplings in the model can be different for each bond or site. Examples are disordered systems, with randomly chosen couplings such as spin glasses,

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```

<LATTICEGRAPH name = "depleted inhomogeneous square lattice">
  <FINITELATTICE>
    <LATTICE dimension="2"/>
    <EXTENT dimension="1" size="L"/>
    <EXTENT dimension="2" size="L"/>
    <BOUNDARY type="periodic"/>
  </FINITELATTICE>
  <UNITCELL>
    <VERTEX/>
    <EDGE>
      <SOURCE vertex="1" offset="0 0"/>
      <TARGET vertex="1" offset="0 1"/>
    </EDGE>
    <EDGE>
      <SOURCE vertex="1" offset="0 0"/>
      <TARGET vertex="1" offset="1 0"/>
    </EDGE>
  </UNITCELL>
  <INHOMOGENEOUS><VERTEX/></INHOMOGENEOUS>
  <DEPLETION>
    <VERTEX probability="DEPLETION" seed="DEPLETION_SEED"/>
  </DEPLETION>
</LATTICEGRAPH>

```

Fig. 1. The definition of a square lattice with one site (vertex) per unit cell and bonds (edges) only to nearest neighbors. First the dimension, extent, and boundary conditions of the Bravais lattice are described in the <FINITELATTICE> element, then the unit cell including the bonds in the lattice is defined. New features in release 1.3. include inhomogeneity and depletion.

or systems in spatially varying trapping potentials, such as optical lattices in harmonic traps. Inhomogeneities can be specified for vertices (sites) and edges (bonds), either for all (such as for all vertices in figure 1), or only for one type of vertex or edge.

The other new feature is depletion of a lattice, where a fraction of sites or bonds is randomly removed from a lattice. Currently only site depletion is implemented, but additional types of depletion can be added easily if the need arises [15]. In the example in figure 1, the fraction of depleted sites is specified to be passed in the DEPLETION input parameter, and the random number generator seed DEPLETION_SEED can be changed to give different random realizations of the depletion pattern.

2.1.2. Model definitions

Figure 2 shows the definition of the Hamiltonian of a bosonic Hubbard model in a harmonic trap

$$H = -\mu \sum_i n_i + \frac{U}{2} \sum_i n_i(n_i - 1) - t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + \frac{K}{2} \sum_i (x_i^2 + y_i^2). \quad (1)$$

The first new feature of release 1.3, shown in this example, is the ability to specify composite site and bond operators, such as the `double_occupancy` site term or the `boson_hop` bond term. These site and bond operators can be used in the specification of the model and of measurements.

The other new feature, also shown in the example, is the ability, in conjunction with the specification of an inhomogeneous

```

<BASIS name="boson">
  <SITEBASIS>
    <PARAMETER name="Nmax" default="infinity"/>
    <QUANTUMNUMBER name="N" min="0" max="Nmax"/>
    <OPERATOR name="bdag" matrixelement="sqrt(N+1)">
      <CHANGE quantumnumber="N" change="1"/>
    </OPERATOR>
    <OPERATOR name="b" matrixelement="sqrt(N)">
      <CHANGE quantumnumber="N" change="-1"/>
    </OPERATOR>
    <OPERATOR name="n" matrixelement="N"/>
  </SITEBASIS>
</BASIS>

<SITEOPERATOR name="double_occupancy" site="x">
  n(x)*(n(x)-1)/2
</SITEOPERATOR>

<BONDOPERATOR name="boson_hop" source="x" target="y">
  bdag(x)*b(y)+bdag(y)*b(x)
</BONDOPERATOR>

<HAMILTONIAN name="trapped boson Hubbard">
  <PARAMETER name="mu" default="0"/>
  <PARAMETER name="t" default="1"/>
  <PARAMETER name="U" default="0"/>
  <PARAMETER name="K" default="0"/>
  <BASIS ref="boson"/>
  <SITETERM site="i">
    -mu*n(i) + U*double_occupancy(i) + K/2*((x-L/2)^2 + (y-L/2)^2)
  </SITETERM>
  <BONDTERM source="i" target="j">
    -t*boson_hop(i,j)
  </BONDTERM>
</HAMILTONIAN>

```

Fig. 2. The definition of a bosonic Hubbard Hamiltonian (1) in a harmonic trap. After describing the local basis for each site and operators acting on it, the first new feature in release 1.3 is the ability to define composite site and bond operators, such as the double occupancy and bosonic hopping terms, which are then used in the definition of the Hamiltonian.

lattice, to use site-dependent couplings, such as the harmonic trapping potential K which depends on the x and y coordinates of the site. This feature has been used for the simulation of cold bosonic gases in optical lattices [16].

2.2. Future plans

The immediate goal for release 1.4 will be to add multi-site interaction terms and measurements, such as ring exchange terms.

With the experience gained in using common file formats for several years across a number of different applications, we next plan to design more widely used common formats, such as standard formats for results of Monte Carlo simulations that have been defined at a workshop in September 2006.

3. Libraries

The ALPS libraries are the foundation of all the ALPS applications, providing functionality common to all of

them, such as file I/O, expression evaluation, parallel job scheduling, or the statistical analysis of Monte Carlo measurements. These libraries make full use of object-oriented and generic programming techniques [18], which allows them to be very flexible without losing any performance compared to FORTRAN programs.

3.1. New features

The new library features are mainly hidden from the application users, providing support for the new features in the input files, discussed above, or providing support for new features in the applications, such as translational symmetries in the diagonalization codes, and the ability to define custom measurements, which will be discussed below.

One new feature that should be mentioned explicitly is the inclusion of random number generators in the expression library. Expressions for couplings and other parameters can make use of new functions `random()`, `normal_random()`, and `integer_random(n)` to obtain uniform random numbers in the interval $[0, 1)$, normally distributed random numbers or integer random numbers between 0 and n . This feature is most useful in conjunction with inhomogeneous lattices to define disordered models.

Another change to be mentioned is that since the parsing of command line options to the application is now handled by the Boost program options library [17], multi-letter command line options now need to be preceded by two hyphens as in `--Tmin`, instead of the previous usage `-Tmin`.

3.2. Future plans

Code from the ALPS libraries has recently been used in the development of Boost [17] libraries. These include optimizations to the Boost.Serialization library, new features for the Boost.Random library, a proposed Boost.MPI library and a Boost.Accumulator library for statistical estimates. Once accepted in the peer review process, and published in a future Boost release, the ALPS codes will be changed to use these Boost libraries. The ALPS libraries will then contain less general purpose codes (which will have been moved to Boost) and will be more focused on domain-specific libraries for the simulation of quantum models.

4. Applications

In addition to common libraries, the ALPS project includes a number of ready to use applications implementing the most important unbiased algorithms for quantum many body systems. The applications all share the same file formats, simplifying their use, reducing the learning curve, and enabling the easy investigation of a model with more than one method. Tutorials on the use of the applications are included with the sources that can be found on the ALPS web page [2].

4.1. Exact diagonalization

The existing exact diagonalization [11, 19] programs `sparseddiag` and `fulldiag` have been substantially improved. `sparseddiag` calculates the ground state and low lying excited states of quantum lattice models using the Lanczos [20] algorithm, while `fulldiag` calculates the complete spectrum of quantum lattice models and from it all thermodynamic properties.

The first major improvement is the use of translation symmetry to reduce the Hilbert space dimension. This speeds up the calculations and allows larger systems to be calculated. In addition, by calculating the energy eigenvalues separately for each momentum, the momentum-resolved excitation spectrum can be calculated.

The second new feature is the possibility to define custom measurements of averaged or local site- and bond operators, as well as arbitrary 2-point correlation functions. As an example, for the inhomogeneous bosonic Hubbard model of figure 2, one can specify the measurement of the average double occupancy, local density, density correlations, and Green's function by defining the following input parameters, which use the definitions of site and bond operators provided with the model:

```
MEASURE_AVERAGE[Double] = double_occupancy
MEASURE_LOCAL[Local density] = n
MEASURE_CORRELATION[Density correlation] = n
MEASURE_CORRELATION[Green function] = "bdag:b"
MEASURE_STRUCTURE_FACTOR[Spin Str Fact] = Sz
```

In the future we plan to support point group symmetries and to add the calculation of dynamical correlation functions.

4.2. Classical Monte Carlo

The Monte Carlo program for classical magnets employing local and cluster updates [21] has been extended according to wishes of several users. The most notable new features are the possibility to specify single ion anisotropies and anisotropic interactions.

4.3. Quantum Monte Carlo

The quantum Monte Carlo programs have also been updated in release 1.3.

The “looper” program using the loop cluster algorithm [7, 22] in a stochastic series expansion [23] (SSE) and path-integral representation for quantum magnets has been replaced with a new version, offering 40–80% speed increase and supporting longitudinal and transverse magnetic fields as well as single ion anisotropies.

The directed loop QMC program [24] in an SSE representation for bosonic and magnetic quantum lattice models has been extended to offer also the “Locally optimal worm algorithm” (LOWA) [25] updates.

The worm algorithm [26] program has been updated to allow nonlocal interactions [27].

All QMC program have been extended by new measurements, including correlation functions, structure factors, and stiffness or superfluid density. In addition, the same custom measurements as discussed above for exact diagonalization can be used in these codes, as long as the measurements are diagonal in the chosen basis. The looper program additionally measures local susceptibilities and transverse magnetization.

4.4. Density Matrix Renormalization Group

In addition to the DMRG [9–11] program for *noninteracting* particles (an adaptation of the program in Refs. [28,29] to the ALPS libraries), release 1.3 contains a new DMRG program for interacting many body systems, with the ability to calculate local quantities and two-point correlation functions.

4.5. Tools

Release 1.3 adds a database tool, to archive a collection of simulation results, and to allow fast and efficient extraction and evaluation of results. The tool, based on the SQLite [30] database is easy to use, based on a simple flat file database and does not require to set up a complex database application.

5. License

The ALPS software is distributed under the ALPS library [31] and application [32] licenses, which have remained unchanged. The use of the codes is free for non-commercial applications but carries a citation requirement to publications, such as the current one, describing the libraries and codes. In addition, besides the required citation of the publication describing the ALPS application, users are encouraged to cite the publication describing the algorithm used in the applications.

6. Distribution, outreach development

The ALPS web page [2] is the central information repository of the ALPS collaboration. It makes source codes of the ALPS libraries and applications available, provides access to the documentation, and distributes information about the mailing lists, new releases, and workshops.

For this release we have replaced the static web page by a Wiki system [33], which enables developers and users to easily and quickly add new contents and improve the instructions and tutorials on the web page.

Another new feature is cdALPS [34] by G. Pawłowski, a bootable Knoppix Linux ALPS CD, which allows to run the ALPS tutorials and simple ALPS codes on a PC without installing the full ALPS software.

Development of the ALPS libraries and applications is coordinated through both mailing lists and semi-annual developer workshops. Interested researchers are invited to

join the mailing list and participate in the workshops.

7. Future plans

7.1. New application

The following new applications are planned for future releases:

- A series expansion [35] code for both perturbation series and high temperature series in release 1.4
- Also in release 1.4, the addition of generalized sampling algorithms, such as the quantum version [8] of the Wang-Landau algorithm [36] and optimized ensemble methods [37] to the quantum Monte Carlo algorithms to obtain thermodynamic quantities over large temperature ranges.
- Implementation of parallel tempering [38] for the classical and quantum Monte Carlo algorithms including feedback-optimized temperature sets [39].
- A QMC algorithm in the valence bond representation for quantum spin systems [40]
- A continuum QMC program for bosons, implementing the continuous space worm algorithm [41].

7.2. Realistic model: interface to band structure codes

Also planned for release 1.4 is an interface of the ALPS applications to band structure codes. Instead of running simulations on phenomenological toy models, such as a simple Heisenberg model with only a few different couplings, it will be possible to run the ALPS applications on a complex, realistic model obtained from ab-initio band structure calculations. In the past this was done manually, e.g. in reference [42], the exchange couplings determined in an LDA+U calculation [43] using the Lichtenstein method [44] were used to manually prepare input files for QMC simulations using the loop algorithm [7].

Release 1.4 of ALPS will contain tools to automate such calculations, based on a standard XML I/O format for band structure codes developed by T. Schulthess and M. Summers at the Oak Ridge National Laboratory. As an example of such an automated calculation using a prototype tool by A. Kozhevnikov, we show in figure 3 a comparison of experimental measurements on the spin ladder compound SrCu_2O_3 [45] with automated ab-initio simulations (“LDA+U+ALPS”).

7.3. Dynamical mean field theory (DMFT) solvers

In a further stage, we plan to expand the ALPS project to include dynamical mean field theory (DMFT) [46] solvers. We have designed a DMFT framework for QMC solvers and implemented the standard Hirsch-Fye solver [47], as well as two new continuous time solvers [12,48]. The first application of the framework, a careful comparison of the performance of the three solvers [12,47,48] is in prepara-

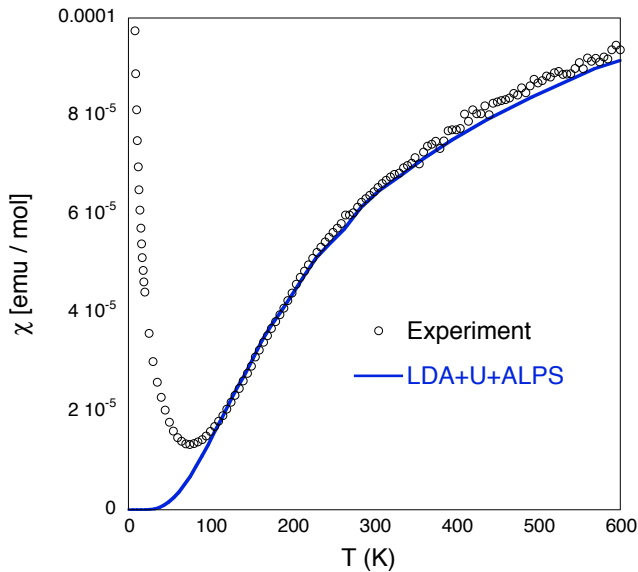


Fig. 3. Comparison of experimental measurements on the spin ladder compound SrCu_2O_3 [45] with automated ab-initio simulations using “LDA+U+ALPS”. The deviation at low temperature is due to impurities in the experimental sample, causing a Curie-Weiss like divergence at low temperatures. The dominant couplings are an intra-chain coupling $J = 162\text{meV}$ and an inter-chain coupling $J_{\perp} = 76\text{meV}$

tion [49]. Work is in progress to expand the framework to include ED and DMRG based solvers, and we expect a public open-source release of the first codes soon. Interested researchers can contact us to participate in the development or to obtain pre-release versions of the codes.

8. Conclusions

The ALPS project is continuously evolving. Researchers interested in announcements of new releases, information about workshops, or in contributing to the ALPS project are encouraged to sign up to the mailing lists on our web page [2].

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