The ALPS project release 2.0: Open source software for strongly correlated systems

B. Bauer[1] **L. D. Carr**[2] **H.G. Evertz**[3] **A. Feiguin**[4] **J. Freire**[5] **S. Fuchs**[6] **L. Gamper**[1] **J. Gukelberger**[1] **E. Gull**[7] **S. Guertler**[8] **A. Hehn**[1] **R. Igarashi**[9,10] **S.V. Isakov**[1] **D. Koop**[5] **P.N. Ma**[1] **P. Mates**[1,5] **H. Matsuo**[11] **O. Parcollet**[12] **G. Pawłowski**[13] **J.D. Picon**[14] **L. Pollet**[1,15] **E. Santos**[5] **V.W. Scarola**[16] **U. Schollwöck**[17] **C. Silva**[5] **B. Surer**[1] **S. Todo**[10,11] **S. Trebst**[18] **M. Troyer**[1]‡ **M. L. Wall**[2] **P. Werner**[1] **S. Wessel**[19,20]

[1]Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
[2]Department of Physics, Colorado School of Mines, Golden, CO 80401, USA
[3]Institut für Theoretische Physik, Technische Universität Graz, A-8010 Graz, Austria
[4]Department of Physics and Astronomy, University of Wyoming, Laramie, Wyoming 82071, USA
[5]Scientific Computing and Imaging Institute, University of Utah, Salt Lake City, Utah 84112, USA
[6]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany
[7]Columbia University, New York, NY 10027, USA
[8]Bethe Center for Theoretical Physics, Universität Bonn, Nussallee 12, 53115 Bonn, Germany
[9]Center for Computational Science & e-Systems, Japan Atomic Energy Agency, 110-0015 Tokyo, Japan
[10]Core Research for Evolutional Science and Technology, Japan Science and Technology Agency, 332-0012 Kawaguchi, Japan
[11]Department of Applied Physics, University of Tokyo, 113-8656 Tokyo, Japan
[12]Institut de Physique Théorique, CEA/DSM/IPhT-CNRS/URA 2306, CEA-Saclay, F-91191 Gif-sur-Yvette, France
[13]Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland
[14]Institute of Theoretical Physics, EPF Lausanne, CH-1015 Lausanne, Switzerland
[15]Physics Department, Harvard University, Cambridge 02138, Massachusetts, USA
[16]Department of Physics, Virginia Tech, Blacksburg, Virginia 24061, USA
[17]Department for Physics, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, University of Munich, 80333 Munich, Germany
[18]Microsoft Research, Station Q, University of California, Santa Barbara, CA 93106, USA
[19]Institute for Solid State Theory, RWTH Aachen University, 52056 Aachen, Germany

‡ Corresponding author: troyer@comp-phys.org

[20]Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Abstract. We present release 2.0 of the ALPS (Algorithms and Libraries for Physics Simulations) project, an 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. The code development is centered on common XML and HDF5 data formats, libraries to simplify and speed up code development, common evaluation and plotting tools, and simulation programs. The programs enable non-experts to start carrying out serial or parallel 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), the density matrix renormalization group (DMRG) both in a static version and a dynamic time-evolving block decimation (TEBD) code, and quantum Monte Carlo solvers for dynamical mean field theory (DMFT). The ALPS libraries provide a powerful framework for programers to develop their own applications, which, for instance, greatly simplify the steps of porting a serial code onto a parallel, distributed memory machine. Major changes in release 2.0 include the use of HDF5 for binary data, evaluation tools in Python, support for the Windows operating system, the use of CMake as build system and binary installation packages for Mac OS X and Windows, and integration with the VisTrails workflow provenance tool. The software is available from our web server at `http://alps.comp-phys.org/`.

1. Introduction

In this paper we present release 2.0 of the ALPS project (Algorithms and Libraries for Physics Simulations), an open source software development project for strongly correlated lattice models. This paper updates the publications on the previous releases [1, 2] to include changes and new features in version 2.0.

Quantum fluctuations and competing interactions in quantum many body systems lead to unusual and exciting properties of strongly correlated materials such as quantum magnetism, high temperature superconductivity, heavy fermion behavior, and topological quantum order. The 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 two decades have seen tremendous progress in the development of algorithms, including refinements to existing numerical algorithms, such as exact diagonalization [3], the density matrix renormalization group [4, 5, 6, 7] and (quantum) Monte Carlo (QMC) techniques, as well as the advent of a new class of variational approaches based on tensor network states [8, 9, 10, 11, 12]. Some of the algorithmic refinements have led to computational speedups of many orders of magnitude, such as the development of non-local update schemes [13, 14] in QMC methods [15, 16, 17, 18, 19, 20, 21, 22], the sampling of extended ensembles [23, 24, 25, 26, 27, 28], or the continuous-time approach to quantum impurity problems [29, 30, 31, 32, 33]. These advances often come at the cost of 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 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. At the same time, the use of numerical approaches is increasing.

2. The ALPS project

2.1. Overview

The ALPS project aims to overcome the problems posed by the growing complexity of algorithms and the specialization of researchers to single algorithms through an open-source software development initiative. Its goals are to simplify the development of new codes through libraries and evaluation tools, and to help users with "black box" codes of some of the most popular algorithms. To achieve these goals the ALPS project provides:

- **Standardized file formats** based on XML [34] and HDF5 [35] to simplify exchange, distribution and archiving of simulation results, and to achieve interoperability between codes.
- **Evaluation tools** for reading, writing and post-processing simulation results, including the creation of 2D and 3D plots.
- **Libraries** for common aspects of simulations of quantum and classical lattice models, to simplify code development and allow implementation on a variety of serial and parallel platforms.
- A set of **applications** covering the major algorithms. These are useful for: *theoreticians* who want to test theoretical ideas or new algorithms for lattice models and to explore their properties, *experimentalists* trying to fit experimental data to theoretical models to obtain information about the microscopic properties of materials, and *students* learning computational physics and many-body theory.
- A **build system** allowing ALPS to be built on Linux, MacOS X, Windows, and supercomputing platforms, and the creation of simple binary installers.
- An extensive set of **tutorials** teaching the use of the ALPS libraries and the various applications.
- **License** conditions [36, 37] that encourage researchers to contribute to the ALPS project by gaining scientific credit for use of their work.
- **Outreach** through a web page [38], mailing lists, and workshops to distribute the results and to educate researchers both about the algorithms and the use of the applications.

- **Improved reproducibility** of numerical results by publishing source codes used to obtain published results and by integration with the VisTrails [39] provenance enabled workflow system.

In contrast to other fields, where open-source development efforts started decades ago, we can directly build our design on recent developments in computer science, especially:

- XML[34] (eXtensible Markup Language) and HDF5[35] (Hierarchical Data Format version 5) as portable data formats supported by a large number of standard tools
- generic and object oriented programming in C++ to achieve flexible but still optimal codes
- OpenMP[40] and MPI[41] for parallelization on shared memory machines, clusters, and high performance supercomputers.

2.2. New features in version 2.0

The specific new features in version 2.0 are:

- CMake build system [42], simplifying configuration and enabling ALPS to be built on Windows.
- Binary installer packages for MacOS X and Windows.
- Using the binary file format HDF5 [35] in addition to XML, which is much faster and needs less space.
- More flexible and powerful evaluation tools using Python.
- A revised and substantially faster version of the directed loop quantum Monte Carlo (QMC) code `dirloop_sse`, and two new applications: QMC solvers for dynamical mean field theory (`dmft`) and a time-evolving block decimation code (`tebd`) for the dynamics of one-dimensional quantum systems.
- Integration with the VisTrails workflow provenance system [39].
- An expanded set of tutorials, and completely new tutorials using Python and VisTrails.

3. Building and Installing ALPS

3.1. Build system

ALPS 2.0 uses CMake [42], which is more flexible and portable than the previously used `autotools`. All aspects of the build process are controlled by CMake variables, which can be easily changed in several ways, including a graphical user interface. This allows the user a large degree of customization of the ALPS installation. Furthermore, CMake supports the automatic creation of binary installation packages and building ALPS on Windows – two often requested features. A snapshot of the build instructions at the time of the release are included in the source distribution.

3.2. Building ALPS from source

Details about building ALPS from source and the required tools and libraries are discussed in Appendix C. This is the recommended way of building ALPS on Unix and Linux systems or if one wants to use specific BLAS libraries or Python interpreters on MacOS or Windows. Updated instructions as operating systems change will be made available on the ALPS web page [38].

3.3. Binary Installation Packages

To simplify installation on Mac OS X and Windows, we provide CMake-generated binary installation packages for these operating systems. To take advantage of all features of ALPS we recommend the user to download and install a binary installer for VisTrails [39] in addition to the ALPS installers. On both operating systems the PATH variable should be adjusted to include the directory containing the ALPS binaries. The Windows installer gives one the option to do so automatically. The default installation directory on Mac OS X is `/opt/alps/bin` and on Windows `C:\Program Files\ALPS\bin` on 32-bit versions and `C:\Program Files (x86)\ALPS\bin` on 64-bit versions, respectively.

Source and binary installation packages for Mac OS X using macports [43] and for Linux using Ubuntu and Debian package managers will be made available in the near future.

3.4. LiveALPS

For Linux we additionally provide an ISO disk image, called LiveALPS, of a full Linux distribution with ALPS preinstalled. Based on a remastered CD-release of Knoppix [44] it is ready to use on a PC without special configuration. While it can be burned to a DVD we recommend using it with a USB flash drive for performance reasons. This solution is especially useful for Linux users that want to try ALPS, in summer schools, or in lectures.

4. Data formats

The most fundamental 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, reduce the learning curve, 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.

4.1. XML

The ISO standard XML [34] was chosen in ALPS version 1 [1, 2] 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 [45] to describe

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

An introduction to XML and the ALPS XML formats is given in Appendix D, and a detailed specification of the formats is provided on our web pages [38, 45].

4.2. HDF5

We now complement XML by the widely used Hierarchical Data Format 5 (HDF5) [35], a de-facto standard for writing large binary files in a portable, machine-independent way. HDF5 is directly supported by many visualization and data analysis tools and a wide array of tools are available for C, C++, Fortran, Python, and other languages. In ALPS, HDF5 is now used as the default output format for simulation data. This approach is significantly faster than writing to text-based formats when large files need to be written. On-the-fly compression of binary data further reduces file size.

The ALPS HDF5 files store simulation parameters, the detailed results of Monte Carlo simulations, spectra and expectation values of exact diagonalization and DMRG simulations, and time evolutions in the TEBD code. ALPS comes with a library of C++ and Python functions to load these results, but they can also be read with any other tool supporting HDF5. The exact schema of the HDF5 files is available on the ALPS web page [38]. For backward compatibility with users' evaluation tools, the simulation codes accept a `--write-xml` command line option to also write all results in XML.

The implementation of HDF5 capabilities within ALPS is split into two layers. The lower layer implements a generic and general-purpose C++ interface to the C HDF5 library. This layer is not tied to other parts of the ALPS library and can therefore be used by user code that is otherwise independent from ALPS and its file formats. The functions of this library are also exposed to Python, and can thus be used not only from C++ codes but also from Python scripts. On top of that, the specific file formats used by the ALPS library and applications are implemented in the respective components of the ALPS library.

5. ALPS Libraries

Main developers: L. Gamper, E. Gull. A. Hehn, B. Surer, S. Todo and M. Troyer.

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

- an XML parser and output stream to read and write the ALPS XML files.

- a HDF5 library to read and write HDF5 files
- an expression library to manipulate and evaluate symbolic expressions.
- a scheduler for the automatic parallelization of Monte Carlo simulations and other embarrassingly parallel applications, implementing load balancing and checkpointing [46].
- a lattice structure library for the creation of arbitrary graphs and Bravais lattices from XML input.
- a model library for the construction of basis sets, operators and Hamiltonians from XML input.
- the "alea" library for the statistical analysis and evaluation of Monte Carlo data including a binning analysis of errors and jackknife analysis of cross-correlations [46].
- a serialization library "osiris" for the serialization of C++ data structures, used for writing program checkpoints and portable binary result files [46].

These libraries make full use of object oriented and generic[47] programming techniques, thus being flexible while still not losing any performance compared to FORTRAN programs. To give just one example, the lattice library, implemented generically using C++ template features, is based on the Boost Graph Library[48, 49] (BGL) and does not restrict the user to a specific data structure as in C or Fortran libraries. Instead the application programmer can choose the data structure best suited for the application, and as long as the data structure provides the BGL graph interface, the ALPS lattice library can construct the lattice from the XML description.

6. Evaluation Tools in Python

Main developers: B. Bauer, L. Gamper, J. Gukelberger, P.N. Ma, O. Parcollet, B. Surer, M. Troyer, and M. L. Wall.

The previous versions of ALPS had very limited data evaluation capabilities that were restricted to extracting plots from collections of XML files using XSLT. This is remedied in ALPS 2.0 by basing data evaluation on the powerful Python language [50]. Python is an easy-to-learn, interpreted, object-oriented language allowing interactive analysis of data and arbitrary complex evaluations. Some brief examples of the Python language as well as the pyalps Python package new to ALPS 2.0 can be found in Appendix B.

We provide a complete set of library functions to write and read ALPS files and a number of useful functions to evaluate the simulation results and to make plots. In particular, the ALPS classes for the recording and evaluation of Monte Carlo data are all exported from C++ to Python, enabling an easy binning analysis [51] and jackknife analysis of Monte Carlo data. Two-dimensional plots are created using the widely available Python matplotlib package [52] or by using ALPS functions to write grace [53] or gnuplot [54] input files. Creation of 3D graphs is supported through VisTrails and the Visualization ToolKit (VTK) [55] VisTrails modules.

6.1. The Python language

Python [50] is an open-source, high-level, object-oriented interpreted programming language developed with a focus on portability and high productivity. This is achieved with a clear syntax and extensive standard libraries. A wealth of material is available for learning the language, including its own extensive standard documentation and several books[56, 57].

Python is an interpreted language, meaning that the source code is executed without an intermediate compilation step. This allows for interactive use, and easy analysis of simulation data. It also is simplifies code development and exchange, in particular since using an interpreted language also often improves the portability of the resulting code.

In addition to the Python standard library, the PyLab environment, which consists in particular of the NumPy [58], SciPy [59] and matplotlib [52] libraries, offers powerful tools for numerical calculations and plotting. This makes Python particularly suitable for the data analysis part of the overall ALPS workflow. Wherever possible, the data types used in the pyalps package are built on top of the NumPy data types, allowing direct use of the PyLab libraries.

Python programs can interoperate with code written in a different language. As an example, a low-level numerical method could be implemented in C/C++ for performance reasons but still be called from a high-level Python code. This can be significantly simplified by using the Boost.Python [49] library. Specifically, this library provides a simple interface to export C++ functions and classes to Python while taking care of Python internals such as memory management. We make use of this library to export parts of the ALPS library to Python in the pyalps package.

6.2. The pyalps package

ALPS 2.0 contains a package of Python modules for interfacing the low-level ALPS code to Python and vice versa, running simulations, and evaluation and post-processing of data. This package is known as pyalps. The advantages of using Python versus exclusively using low-level code for the above tasks are manifold. For example, Python's large standard library and ability to easily interface with low-level code allow for great flexibility in post-processing of data. Also, the use of Python facilitates use of the VisTrails workflow provenance tool, as VisTrails is written in Python.

Pyalps includes functions to write the xml files read by most applications, and additional functions to write special input files for applications with non-xml interfaces such as `dmft` and `tebd`. It also includes functions to run applications with specified input files both in series and in parallel. An example of the preparation of input files and running a simulation using pyalps is shown in Fig. 5.

Once the simulation has been run we must extract and evaluate data from it. At the heart of the pyalps evaluation tools is the `DataSet` class. A `DataSet` has as members `x` and `y` which are NumPy arrays containing numerical data. A `DataSet` also has a member `props` which is a dictionary – one of the built-in types of Python – of metadata describing the numerical data. The presence of the metadata allows for complex evaluations, for example when dealing with many `DataSet`s from a parameter scan.

Using Boost.Python, large parts of the ALPS alea library for Monte Carlo observables are exported to Python. This allows the user to write Monte Carlo applications in Python while profiting from the full functionality of the ALPS C++ libraries. In addition, this allows the definition of numerical data types in Python which carry full statistical information. These types allow calculations with the syntax of normal floating-point numbers, but will perform a full error analysis. We also provide functions to read HDF5 files into a `DataSet`. Wrapper functions around matplotlib for plotting of data stored in `DataSet`s help the user by, e.g., automatically setting axis labels or legends from the metadata.

7. 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. All applications from ALPS 1.3, with the exception of the single particle DMRG demonstration program, have been retained in ALPS 2.0. They continue to work in the same way, with minor bug fixes and patches for incompatibilities, and we have added a number of new applications in version 2.0.

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 [38].

7.1. Exact diagonalization

The exact diagonalization codes have been optimized for flexibility and not the highest performance or the goal to reach the biggest system sizes.

The codes make use of conserved quantum numbers, such as particle number or magnetization, and use 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 user may also specify 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 D6, 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[Density Structure Factor] = n
```

7.1.1. Sparse diagonalization code `sparsediag`*,* main developer: M. Troyer

`sparsediag` calculates the ground state and low lying excited states of quantum lattice models using the Lanczos [3] algorithm.

7.1.2. Full diagonalization code `fulldiag`*,* main developer: M. Troyer

`fulldiag` calculates the complete spectrum of quantum lattice models and from it all thermodynamic properties. Access to the complete spectrum allows the calculation of all thermodynamic properties and of the temperature dependence of any measurement specified by the user.

7.2. Classical Monte Carlo simulations

7.2.1. Classical Monte Carlo codes for spin models `spinmc`*,* main developer: M. Troyer

`spinmc` is a classical Monte Carlo code for classical magnets employing local and cluster updates [13, 14]. Supported models are Ising, XY, Heisenberg, and Potts models with isotropic and anisotropic interactions and magnetic fields.

7.3. Quantum Monte Carlo simulations

7.3.1. The looper code, main developer: S. Todo

The `loop` program implements the loop cluster algorithm [15, 18, 19, 21], a generalization of the classical cluster updates [13, 14] to quantum systems in both a path integral and a stochastic series expansion (SSE) representation [60, 17]. It supports isotropic and anisotropic models of quantum magnets in transverse and longitudinal fields.

7.3.2. The directed loop algorithm code `dirloop_sse`*,* main developer: S. Isakov and L. Pollet

The `dirloop_sse` code in ALPS 2.0 is a completely new and improved implementation of the directed loop QMC algorithm [20, 22], replacing the previous one in ALPS 1.2 and 1.3. It is ideal for spin models in magnetic fields, frustrated spin models, and hard-core boson models.

7.3.3. The worm algorithm code `worm`*,* main developers: S. Trebst and M. Troyer
The `worm` code implements the worm algorithm [16] and is ideal for bosonic models.

7.3.4. The extended ensemble code `qwl`*,* main developers: M. Troyer and S. Wessel
The `qwl` code is an extended ensemble QMC program using a generalization of the Wang-Landau[23, 24] algorithm to quantum systems,[25] to obtain thermodynamic quantities over large temperature ranges.

7.4. Density Matrix Renormalization Group (DMRG) algorithms

7.4.1. The `dmrg` *code,* main developers: A. Feiguin (core code) and M. Troyer (ALPS interface)

The `dmrg` code implements the DMRG algorithm [4, 5] to calculate ground states and low-lying excited states of quasi-one dimensional quantum systems. It can also measure arbitrary local quantities and two-point functions.

7.4.2. Time Evolving Block Decimation Code `tebd`*,* main developers: L. D. Carr and M. L. Wall

Release 2.0 contains interfaces to the Open Source TEBD project [61], which is a collection of Fortran libraries using the Time-Evolving Block Decimation (TEBD) algorithm [8, 9] to simulate time evolution of one-dimensional quantum systems. TEBD can also find ground states via imaginary time evolution. The TEBD routines included in ALPS are an updated version of the v2.0 release of Open Source TEBD with improvements for speed and numerical stability.

At present, the TEBD routines can simulate the spin, boson Hubbard, hardcore boson, spinless fermion, and fermion Hubbard models from the ALPS models library. All Hamiltonian parameters are assumed uniform throughout the system. Because TEBD produces wavefunctions, a wide array of observables can be computed including local quantities, two-point correlation functions, entanglement measures, and overlaps between the state at different times. Observables calculated are the z and x magnetizations, their squares, and the $\langle \hat{S}^z_i \hat{S}^z_j \rangle$ and $\langle \hat{S}^x_i \hat{S}^x_j \rangle$ correlations for the spin model, the occupation number, its square, and the $\langle \hat{n}_i \hat{n}_j \rangle$ and $\langle \hat{a}^\dagger_i \hat{a}_j \rangle$ correlation functions for the boson Hubbard, hardcore boson, spinless fermions, and fermion Hubbard models; and, additionally, the magnetization and $\langle \hat{S}^z_i \hat{S}^z_j \rangle$ correlation function for the fermion Hubbard model. All models calculate the energy, von Neumann entanglement entropy of each site, the von Neumann entanglement entropy on each bond, and the overlap of the wavefunction at time t with the state at $t = 0$ (*i.e.*, the Loschmidt echo).

7.5. Dynamical Mean Field Theory QMC Solvers `dmft`

Main developers: S. Fuchs, E. Gull, B. Surer, M. Troyer and P. Werner

Dynamical mean field theory (DMFT) is a method to simulate fermionic lattice systems which approximates the self-energy $\Sigma(k,\omega)$ by a momentum-independent function $\Sigma(\omega)$. For such a "local" self-energy, the diagrammatic structure simplifies considerably and the lattice problem can be mapped onto an impurity problem subject to a self-consistency condition for the bath [62, 63]. The method may be extended from a single-site to a cluster formalism, thereby rendering it controlled in practice [64]. We provide a simple implementation of the DMFT self-consistency loop for general single-site multi-orbital problems. For the solution of the quantum impurity model we provide a legacy Hirsch-Fye QMC code [65] as well as two continuous-time QMC algorithms.

The "interaction expansion" algorithm [29, 30] expands the impurity model partition function in powers of the interaction terms and samples the resulting diagrams stochastically. This method, historically the first continuous-time quantum Monte Carlo impurity solver algorithm, is particularly suitable for the simulation of impurity clusters. The complementary hybridization expansion algorithm [31, 32] expands the impurity model partition function in the impurity-bath hybridization, treating the local (impurity) Hamiltonian exactly. The method is useful to simulate multi-orbital models, since it can easily treat general interaction terms. The current implementation of the ALPS code (both for the interaction expansion and the hybridization expansion) is restricted to (multiorbital) single site and density-density interactions. A detailed description of the ALPS DMFT algorithms is given in Ref. [66].

8. Integration with the VisTrails Workflow and Computational Provenance Tools

Main developers: B. Bauer, J. Freire, L. Gamper, J. Gukelberger, D. Koop, P. Mates, E. Santos, V.W. Scarola, C. Silva, B. Surer and M. Troyer.

8.1. Computational Provenance

ALPS 2.0 seeks to ensure result reproducibility. Provenance (also referred to as history, audit trail, lineage, or pedigree) captures information about the steps used to generate a given result [67, 68]. Such information is crucial in data preservation and determining data quality as well as interpreting, reproducing, sharing, and publishing results. Release 2.0 improves upon previous ALPS versions by using the VisTrails [39] workflow system to record provenance-related information, including algorithm workflows, simulation parameters, and version history to automate reproducibility.

VisTrails is an open-source system that was designed to support exploratory computational tasks such as visualization and data mining while ensuring computational provenance [39, 69]. VisTrails enforces provenance with workflows that allow a capture mechanism and an infrastructure for storage, access, and queries. In Appendix A we present a concise introduction to scientific workflows and VisTrails.

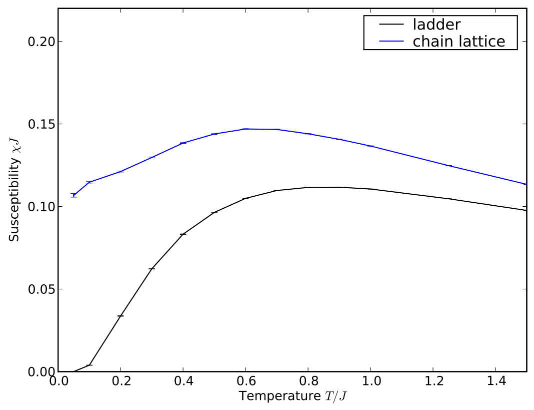


Figure 1. A figure produced by an ALPS VisTrails workflow: the uniform susceptibility of the Heisenberg chain and ladder. Clicking the figure retrieves the workflow used to create it. Opening that workflow on a machine with VisTrails and ALPS installed lets the reader execute the full calculation.

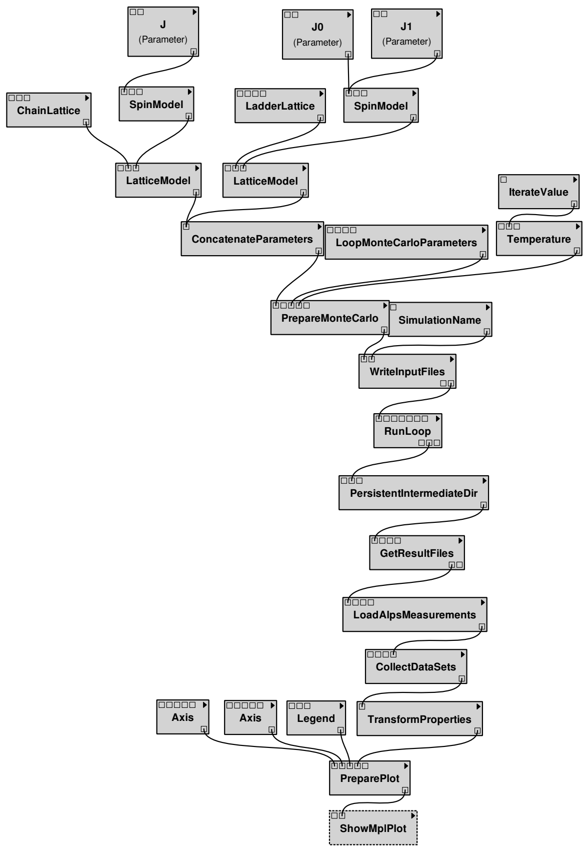


Figure 2. The workflow that created Fig. 1. The workflow image has been created by VisTrails for the specific workflow used to create the exact version shown in the figure. Clicking the figure retrieves the workflow.

8.2. The ALPS VisTrails package

ALPS 2.0 provides a package of modules for VisTrails, built on top of the pyalps package, that allows the user to perform the three major steps of a scientific workflow, namely i) the preparation of input files, ii) the execution of simulations, iii) the analysis and plotting of simulation data. The three groups of modules are intended to integrate seamlessly, but at the same time allow the separate use of each group, which for example allows the user to analyze data with VisTrails that has not been prepared using the ALPS library or file formats.

The design goal of the data analysis modules is to take care of common, repetitive tasks, while at the same time being as flexible as scripts. Common data formats, designed to allow interoperability with the powerful NumPy/SciPy libraries, are used by all modules. A set of self-contained modules are provided for common tasks, such as fitting or various types of plots. A framework of *Transform* modules allows the user to specify arbitrary transformations by providing small Python codes.

The modules for input preparation and data analysis are designed to assist the user in dealing with a large number of simulations. For example, modules are provided to sweep parameter ranges, to combine data from many simulations or to load data from ALPS files and text files. Modules to load data from custom file formats can also easily be implemented.

VisTrails workflows in ALPS 2.0 use descriptive nouns and verbs for the names of modules that execute Python scripts which in turn execute ALPS algorithms in Python or compiled code. Fig. 2 shows an example ALPS workflow that takes input lattice parameters and model definitions (modules described by nouns, such as ChainLattice and LatticeModel), executes the quantum Monte Carlo looper code, and then renders the data (modules described by verbs such as RunLoop and PreparePlot).

The creation of such workflows is explained in a set of tutorials and on the web page. Furthermore, all ALPS tutorials, discussed in the next section, are available as VisTrails workflows, providing an extensive set of examples that can be used as templates for the user's simulations.

This paper already makes use of ALPS 2.0 and VisTrails. Full provenance information for the results in Fig. 1 is available from the URL linked to the figure. Clicking the figure will download the workflow that has been used to prepare the figure and its version history. After installing VisTrails and ALPS, the reader of the paper can redo the full simulation.

ALPS VisTrails is also suitable for data analysis only. For compute-intensive problems requiring computer cluster resources the data analysis within Vistrails is performed by reading the observables from stored result files. Operating in this way is the workflow producing Fig. 3 showing a data collapse of the Binder cumulant in the classical Ising model. The workflow downloads the corresponding result files from a server, loads the Binder Cumulant observable and allows to interactively determine the critical exponents by a parameter exploration. The reader is invited to explore the

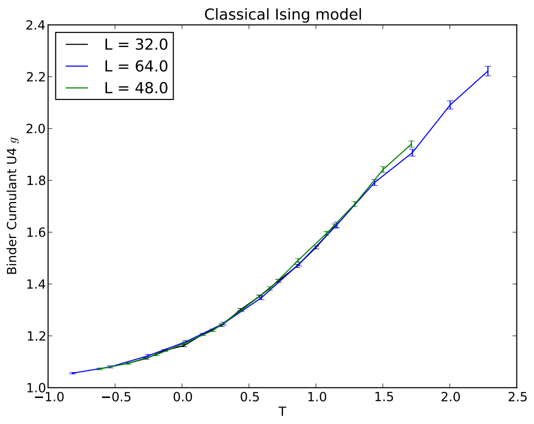


Figure 3. In this example we show a data collapse of the Binder Cumulant in the classical Ising model. The data has been produced by remotely run simulations and the critical exponent has been obtained with the help of the VisTrails parameter exploration functionality.

```
cat > parm << EOF
LATTICE="chain_lattice"
MODEL="spin"
local_S=1/2
L=60
J=1
THERMALIZATION=5000
SWEEPS=50000
ALGORITHM="loop"
{T=0.05;}
{T=0.1;}
{T=0.2;}
{T=0.3;}
{T=0.4;}
{T=0.5;}
{T=0.6;}
{T=0.7;}
{T=0.75;}
{T=0.8;}
{T=0.9;}
{T=1.0;}
{T=1.25;}
{T=1.5;}
{T=1.75;}
{T=2.0;}
EOF

parameter2xml parm
loop --auto-evaluate --write-xml parm.in.xml
```

Figure 4. A shell script to perform an ALPS simulation to calculate the uniform susceptibility of a Heisenberg spin chain. Evaluation options are limited to viewing the output files. Any further evaluation requires the use of Python, VisTrails, or a program written by the user.

sensitivity of the data collapse to the correlation length critical exponent.

9. Tutorials and Examples

Main contributors: B. Bauer, A. Feiguin, J. Gukelberger, E. Gull, U. Schollwöck, B. Surer, S. Todo, S. Trebst, M. Troyer, M.L. Wall and S. Wessel

The ALPS web page [38], which is a community-maintained wiki system and the central resource for code developments, also offers extensive resources to ALPS users. In particular, the web pages feature an extensive set of tutorials, which for each ALPS application explain the use of the application codes and evaluation tools in the context of a pedagogically chosen physics problem in great detail. These application tutorials are further complemented by a growing set of tutorials on individual code development

```
import pyalps
import matplotlib.pyplot as plt
import pyalps.plot

#prepare the input parameters
parms = []
for t in [0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.25, 1.5, 1.75, 2.0]:
 parms.append(
  {
    'LATTICE'  : "chain lattice",
    'MODEL'    : "spin",
    'local_S'  : 0.5,
    'T'        : t,
    'J'        : 1 ,
    'THERMALIZATION' : 5000,
    'SWEEPS'   : 50000,
    'L'        : 60,
    'ALGORITHM'  : "loop"
  }
 )

#write the input file and run the simulation
input_file = pyalps.writeInputFiles('parm2c',parms)
pyalps.runApplication('loop',input_file)

#load the susceptibility and collect it as function of temperature T
data = pyalps.loadMeasurements(pyalps.getResultFiles(prefix='parm2c'),'Susceptibility')
susceptibility = pyalps.collectXY(data,x='T',y='Susceptibility')

#make plot
plt.figure()
pyalps.plot.plot(susceptibility)
plt.xlabel('Temperature $T/J$')
plt.ylabel('Susceptibility $\chi J$')
plt.title('Quantum Heisenberg chain')
plt.show()
```

Figure 5. A Python script to perform an ALPS simulation to calculate the uniform susceptibility of a Heisenberg spin chain, load and evaluate the data, and make a plot.

based on the ALPS libraries.

9.1. Tutorials on Using the ALPS Codes

We provide tutorials and instructions for using ALPS in three ways:

(i) from the command line (without data evaluation and plotting)

(ii) using Python scripts

(iii) and using the VisTrails workflow system.

The input files needed for the tutorials are available on the web page but are also included in the source and binary distributions.

An example for running an ALPS application from the command line is shown in Fig. 4. This example calculates the uniform susceptibility of a quantum Heisenberg spin chain. The same example, containing additional code to evaluate and plot the results using Python is shown in Fig. 5. The workflow using VisTrails is shown in Fig. 2, and its version history in Fig. A3. Following the links in the PDF version of the latter figures retrieves the corresponding vistrail files.

9.2. Tutorials on Writing Codes with ALPS

A second set of tutorials demonstrate how to use ALPS libraries and tools in new simulation codes. We provide examples of how to write a simple Monte Carlo simulation in either Python or C++ and how to integrate it with the ALPS tools. We also demonstrate how a user's code can be easily integrated into the VisTrails workflow system.

10. License

The ALPS libraries are licensed under the ALPS library license [36] and the applications under the ALPS application license [37]. These licenses are modeled after the GNU General Public License (GPL), but contain an additional requirement to cite this paper as well as relevant papers for each of the application codes. These papers need to be cited and the use of ALPS acknowledged in any scientific project that makes use of ALPS. This includes the case when ALPS has only been used to test a scientist's application code.

The detailed license text is included in the files `LICENSE.txt` [36] and `LICENSE-applications.txt` [37]. Any use of ALPS requires citing this paper. These files can be found at the top level of the source distribution and in the directory `share/alps` of the binary distributions. The papers that need to be cited for the use of a specific application are printed to the standard output when that application is run. The list of papers is also included in the file `CITATIONS.txt`. Since some of those references are to preprints we recommend that the ALPS web page [38] is checked for updates.

11. Future Development plans

The ALPS project is a work in progress and development will continue after this release 2.0. Immediate plans for release 2.1 within about a year include the development of more evaluation tools for Monte Carlo simulations and more 2D and 3D plotting functionality.

ALPS 2.1 will also provide support for more programming languages. In addition to the Python support in the current version we plan to add a Fortran library to write the ALPS HDF5 files from Fortran. This will enable the use of the ALPS evaluation tools not only with C++ or Python codes, but also with results of Fortran codes.

A key part of ALPS 2.1 will be a more flexible and optimized scheduler. It will allow the simple integration of ALPS codes into other programs and Python scripts. It is also designed to scale to tens of thousands of CPUs, compared to the current scheduler that scales only to a few thousand CPUs.

Besides improved versions of some of the simulation codes, there will be a new worm algorithm program for optical lattice simulations with millions of lattice sites, and an extension of the DMFT codes to clusters.

ALPS is an open initiative and we welcome contributions from the community.

12. Acknowledgements

We thank A.F. Albuquerque, F. Alet, P. Corboz, P. Dayal, A. Honecker, A. Läuchli, M. Körner, A. Kozhevnikov, S. Manmana, M. Matsumoto, I.P. McCulloch, F. Michel and R.M. Noack, for their contributions to previous versions of ALPS and for useful discussions. We thank D. Abrahams for developing Boost.Python and for his support of the Boost libraries.

We thank all users of the previous versions of ALPS and beta testers of ALPS 2.0, especially J. Alfonsi, S. Aicardi, A. Akande, P. Anders, A. Anfossi, Z. Asadzadeh, R. Bhat, J.H. Brewer, S. Bulut, E. Burovski, G. Carleo, G. Chen, M.D. Costa, M. Dolfi, M. Ferrero, J. Figgins, S. Gazit, U. Gerber, R. Ghulghazaryan, C. Gils, S. Greschner, C. Hamer, J. Hammond, K. Hassan, N. Heine, F.-J. Jiang, R. Jordens, H.G. Katzgraber, B. Keiyh, J. Kim, J. Kolasinski, B. Koopman, F. Körmann, E. Kozik, M.F. Krenn, F. Kruger, M. Laurent, J. Lopes, M. Maik, M. Maksymenko, N. Moran, A. Nunnenkamp, J.D. Peel, S. Pilati, K. Prsa, N. Rahman, M. Rofiq, H. Rønnow, J. Ruostekoski, J. Schnack, N. Schuch, A. Sen, K. Shtengel, J. Single, M. Skoulatos, C. Sliwa, M. Spenke, M. Stoudenmire, V. Tangoulis, A. Taroni, B. Thielemann, M. Tovar, H. Tran, V. Varma, S. Ward, T. Wasiutynski, J. Wen, J. Wilms, H. Wunderlich, F. Xiao, X.Q. Yu, J. Zakrzewski, Z.-X. Zhou, and R. Ziemkiewicz. We thank P. Zoller for the suggestion to provide binary installers.

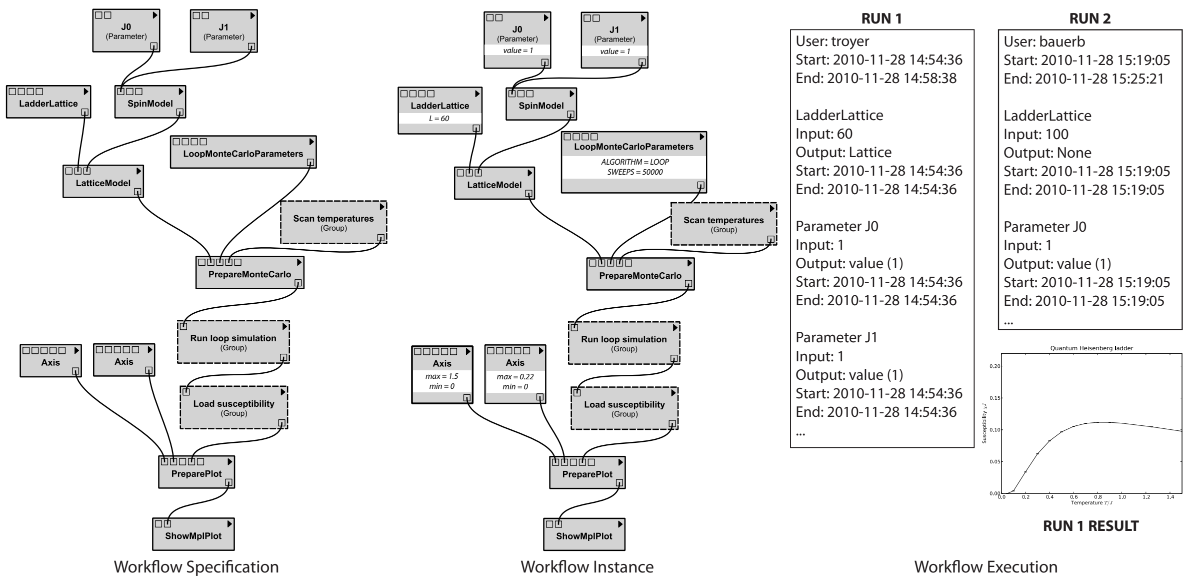
The development of ALPS has profited from support of the Pauli Center at ETH Zürich, the Swiss HP^{2}C initiative, the Kavli Institute for Theoretical Physics in Santa Barbara through NSF grants PHY-0551164 and DMR-0705847, the Aspen Center for Physics, the Swiss National Science Foundation, the Jeffress Memorial Trust, Grant No. J-992, the National Science Foundation under grant PHY-0903457 and DMR-0955707, the Golden Energy Computing Organization at the Colorado School of Mines for the use of resources acquired with financial assistance from the National Science Foundation and the National Renewable Energy Laboratories, the Deutsche Forschungsgemeinschaft through the collaborative research center SFB 602, Japan Society for the Promotion of Science through KAKENHI No. 20540364, Next-Generation Supercomputer Project from MEXT Japan, and a grant from the Army Research Office with funding from the DARPA OLE program.

Work on VisTrails is primarily supported by grants and contracts from the U.S. National Science Foundation, the U.S. Department of Energy, and IBM.

Appendix A. Scientific Workflows and VisTrails

Appendix A.1. Workflows

Workflow systems provide well-defined languages for specifying complex tasks from simpler ones; they capture complex processes at various levels of detail and systematically record the provenance information necessary for automation, reproducibility, and result sharing.



RUN 1

User: troyer
Start: 2010-11-28 14:54:36
End: 2010-11-28 14:58:38

LadderLattice
Input: 60
Output: Lattice
Start: 2010-11-28 14:54:36
End: 2010-11-28 14:54:36

Parameter J0
Input: 1
Output: value (1)
Start: 2010-11-28 14:54:36
End: 2010-11-28 14:54:36

Parameter J1
Input: 1
Output: value (1)
Start: 2010-11-28 14:54:36
End: 2010-11-28 14:54:36
...

RUN 2

User: bauerb
Start: 2010-11-28 15:19:05
End: 2010-11-28 15:25:21

LadderLattice
Input: 100
Output: None
Start: 2010-11-28 15:19:05
End: 2010-11-28 15:19:05

Parameter J0
Input: 1
Output: value (1)
Start: 2010-11-28 15:19:05
End: 2010-11-28 15:19:05
...

Figure A1. The workflow specification (on the left) shows a workflow to calculate the uniform magnetic susceptibility of a quantum Heisenberg spin ladder and plot it as a function of temperature. The workflow instance (in the middle), in addition to the workflow specification, contains value assignments for parameters of the modules. This instance was used to derive the plot in the bottom right. The workflow runs (on the right) consist of information collected while the workflow instance was executed.

We start by introducing basic concepts underlying workflows and provenance along with the basic terminology. Scientific workflows are often used to perform data intensive tasks and are represented as dataflow networks [70] where the execution order is determined by the flow of data through the workflow. Scientific workflow systems offer a number of advantages over programs and scripts for constructing and managing computational tasks. In addition to providing a simple programming model, many systems provide intuitive visual programming interfaces which make them more usable for users who do not have substantial programming expertise. As we discuss below, the structure present in workflow definitions also enables a series of operations and queries that simplify the manipulation and re-use of workflows. From now on, we use the terms scientific workflow, workflow, pipeline, and dataflow interchangeably.

Formally, a *workflow specification* is defined by a tuple $(M, I, O, C, p : O \cup I \rightarrow M)$, where M, I, O, C are, respectively, sets of *modules*, *input ports*, *output ports*, *connections*, and p is a function that assigns a unique module to input and output ports. If $x \in I \cup O$ and $m = p(x)$ then we say that *x is a port of module m* and that m is *the module of x*. The set C of connections is a subset of $O \times I$. In a *connection* $(o, i) \in C$, o is called the *source port* and i is called the *target port*. Furthermore, the module of the source port cannot be the same as the module of the target port. Additionally each port (input or output) has an associated type and a *name* that is unique across the ports of the same module. A *module signature* is defined as a set of pairs, where each pair contains a port name and its type. In addition, each module has a set of *parameters*. Each parameter has a unique *name* across the set of parameters of the same module.

A *workflow instance* consists of a specification combined with bindings that provide values to parameters in the modules. A *workflow run* is the execution of the following algorithm for a workflow instance: each module checks whether all its input ports that are target ports of a connection have a value; if false it waits; if true, the module, according to its semantics, produces output values on its output ports; values that are produced in an output port flow to target ports of all the connections that have that output port as its source port; this algorithm continues until there are no more modules to execute. These concepts are illustrated in Figure A1.

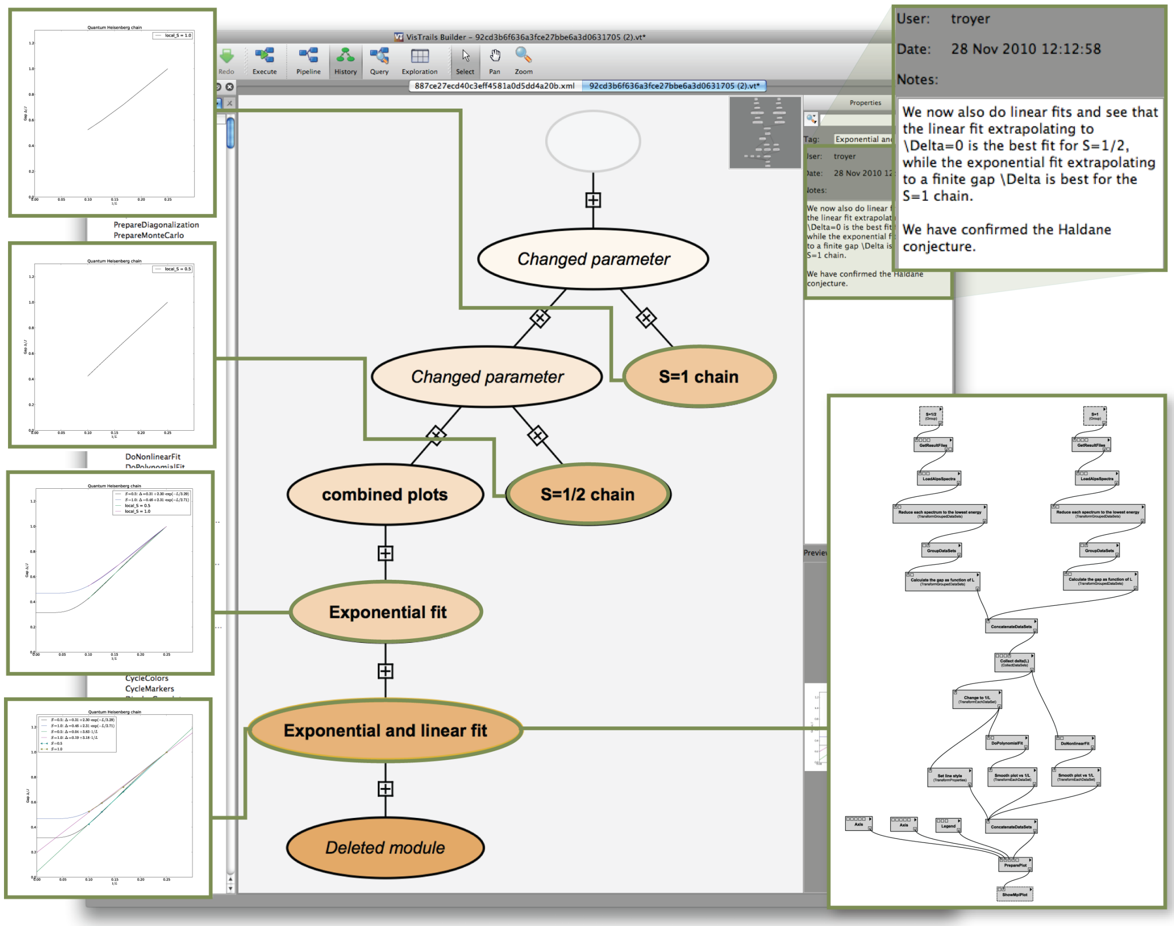
Appendix A.2. Data Provenance

In the context of scientific workflows, data provenance is a record of the derivation of a set of results. There are two distinct forms of provenance [71]: prospective and retrospective. *Prospective provenance* captures the specification of a computational task (i.e., a workflow specification or instance)—it corresponds to the *steps that need to be followed* (or a recipe) to generate a data product or class of data products. *Retrospective provenance* captures the *steps that were executed* (i.e., the workflow run) as well as information about the execution environment used to derive a specific data product—a detailed log of the execution of a computational task.

An important piece of information present in workflow provenance is information about *causality*: the dependency relationships between data products and the processes that generate them. Causality can be inferred from both prospective and retrospective provenance. Data provenance also includes *user-defined information*, such as documentation that cannot be automatically captured but records important decisions and notes. This data is often captured in the form of annotations.

Provenance of Workflow Evolution. Although workflows have been traditionally used to automate repetitive processes, for many exploratory scientific tasks such as data analysis and visualization, change is the norm. As users formulate and test hypotheses, they often need to refine and compare the results of several workflows. VisTrails [39] supports a novel change-based provenance model that treats workflow instances as first-class data products [72, 73]. As a scientist makes modifications to a workflow, the system transparently records those changes (e.g., the addition of a module, the modification of a parameter, etc.) akin to a database transaction log. Note that the change-based model uniformly captures both changes to parameter values and to workflow definitions. This sequence of changes is sufficient to determine the provenance of data products, and it also captures information about how the workflows evolve over time. We refer to this detailed provenance of the workflow evolution as a visual trail, or a *vistrail*.

As Figure A2 illustrates, each node in a vistrail corresponds to a workflow instance and contains value assignments for the module parameters. A series of workflow runs may be associated with a node as well as additional metadata, such as user annotations.



User: troyer

Date: 28 Nov 2010 12:12:58

Notes:

We now also do linear fits and see that the linear fit extrapolating to \Delta=0 is the best fit for S=1/2, while the exponential fit extrapolating to a finite gap \Delta is best for the S=1 chain.

We have confirmed the Haldane conjecture.

Figure A2. Workflow evolution provenance. In this example we have calculated the system size dependence of the spin gap of spin-1 and spin-1/2 Heisenberg chains, first calculating the gap by exact diagonalization and then performing fits to $\Delta(L) = c/L$ and $\Delta(L) = \Delta_0 + c\exp(-L/\xi)$. As expected from the Haldane conjecture the plots show that the first fit is best for the gapless spin-1/2 chain and the second fit is best for the gapped spin-1 chain. Complete provenance of the exploration process is displayed as a history tree with each node representing a workflow instance that generates a plot. Detailed meta-data is also stored including free-text notes made by the scientist, the date and time the workflow was created or modified, an optional descriptive tag, and the user that created it.

A tree-based view of a vistrail allows a scientist to return to a previous version in an intuitive way, to undo bad changes, to compare different workflows, and to be reminded of the actions that led to a particular result. Another important benefit of the change-based provenance model is that it enables a series of operations that simplify the exploration process, in particular, the ability to refine workflows by analogy [74], as well as to visually compare workflows and their results [72].

It is important to note that the provenance of workflow execution and workflow evolution help inform each other, leading to improved methods for using the combined information. Knowing which workflow instances have executed correctly can explain why workflows were updated, and the number of times that an instance has been executed

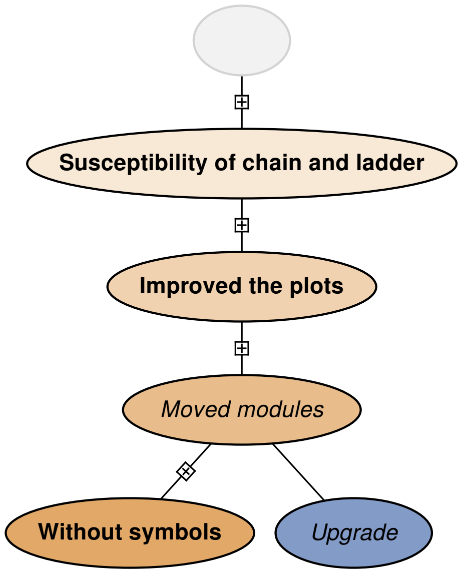


Figure A3. The version history tree of the workflow that created Fig. 1. Each ellipsis corresponds to a version of the workflow, as shown in Fig. 2. Clicking the figure retrieves the vistrail including all workflow versions.

can help highlight important versions of workflows. Similarly, knowing how a workflow evolved can help users debug errors that occur when running modified versions. Change-based provenance from workflow evolution can also speed up runs of similar workflows via caching [75].

Appendix A.3. Caching and persistent storage

One important piece of infrastructure provided by VisTrails is the management of data both used and produced by computational processes, including intermediate results. While parameters and workflow structure may change from execution to execution, many of the intermediate results can be reused without recomputation. Note that with traditional scripts, users must manually record and recall intermediate results, meaning it is often necessary to repeat the entire computation. VisTrails supports efficient exploration of such analyses by automatically caching intermediate results. The results in the cache are identified by the signature of the upstream subworkflow (a hash computed from all of the computations that led to the value). If the signature exists in the cache, we need not compute any of the upstream subworkflow but instead return the value in the cache. If anything in the subworkflow changes, the signature will also change, and VisTrails will recompute the value. VisTrails also allows modules that are not deterministic to be flagged as non-cacheable; note that all modules downstream of such modules must also be recomputed each time.

In addition, VisTrails provides a persistence package to help users manage their data and provide persistent caching. This package provides storage and versioning of input, intermediate, and output data to ensure that workflows are able to access their data. Data is identified by unique IDs rather than file paths, and users can name and annotate the data in order to facilitate searching. The data can be linked to a local disk but is stored in a managed repository to ensure that it is retained. VisTrails will create new versions if data changes, and provides persistent caching using the same signature scheme as in-memory caching. In contrast to the in-memory caching mechanism, a persistent intermediate result can be recalled in later sessions. Using the metadata stored in persistent store and provenance information, it is possible to connect data with the workflows that either used or generated it and vice versa [76]. In addition, users can not only trace data lineage but also retrieve the exact input data—even if that data was changed or removed on the filesystem.

Appendix A.4. Sharing content and reproducible research

One of the goals of the VisTrails system is to facilitate the publication of scientific results. VisTrails and its social workflow repository CrowdLabs greatly simplify the process of packaging workflows and results for publication. By supporting the publication on wikis, web sites, or scientific documents (through LaTeX extensions such as in this paper), this framework allows users to create documents whose digital artifacts (e.g., figures) include a deep caption: detailed provenance information which contains the specification of the computational process (or workflow) and associated parameters used to produce the artifact. Figures 1 and 2 are examples of this mechanism in action: both images were included by using VisTrails directly and clicking on the images will download the workflow with the parameters used to generate them. This workflow can then be used by the reader to reproduce the figures.

CrowdLabs is a social online workflow repository for the VisTrails system. It combines workflow management tools with a scalable infrastructure to allow scientists to collaboratively analyze and visualize data. CrowdLabs is capable of hosting, executing, and serving results from VisTrails workflows, including those that make use of the ALPS VisTrails package. CrowdLabs also leverages provenance information (e.g., workflow/pipeline specifications, libraries, packages, users, datasets and results) to provide a richer sharing experience: users can search and query this information.

VisMashups [77], another component developed on top of VisTrails, is a system for simplifying the creation, maintenance and use of customized workflows. It is also integrated into CrowdLabs and enables users to modify parameters and re-execute workflows from within their web browsers. This provides an entry point for non-experts to explore and interact with complicated simulation workflows. We will develop ALPS tutorials also as VisMashups, enabling the interactive exploration of tutorial problems with the reader's web browser, without the need to install ALPS.

```
# Lists:
tvalues = [0.05, 0.1, 0.2, 0.3, 0.4]
print tvalues[0]

# A list with different types
tvalues = [0.5, 'abc']
```

```
# Creating and accessing a dictionary
parms =
  {
    'LATTICE' : 'chain_lattice',
    'MODEL' : 'spin',
    'local_S' : 0.5,
    'T' : 0.01,
    'J' : 1 ,
    'THERMALIZATION' : 5000,
    'SWEEPS' : 50000,
    'L' : 60,
    'ALGORITHM' : 'loop'
  }

print parms['J']
```

Figure B1. Examples for creating lists and dictionaries in Python.

Appendix B. Python examples

The Python language and its use for the evaluation tools of ALPS are explained in Section 6. In this appendix, we give some examples for the usage of Python and the pyalps package.

Python contains a large number of built-in high-level data types, such as strings, integers, floating point numbers, lists, and dictionaries. The dictionary type in Python is called a `dict`, and is a mutable group of key and value pairs. All the built-in container types in Python can store elements of different type at the same time. The `dict` type is used in ALPS 2.0 to pass metadata about a simulation to the simulation execution commands. An example of this is is shown in Fig. 5, where the parameters for a series of Monte Carlo simulations are stored in the dict `parms` and passed to the `writeInputFiles` function of the pyalps package to write input files for the loop application. Fig. B1 shows examples of how to use lists and dictionaries in Python.

The `def` statement defines a function or method. An example of a simple Python function from the pyalps package is given in Fig. B2. This example also demonstrates the unusual feature of Python that tab indentation is used for block delimiters.

In addition to the procedural programming paradigm, Python supports object-oriented programming. Since the `DataSet` class is a crucial part of the pyalps package, a slightly reduced version is shown as example class in Fig. B3. The declaration of a class is started by the `def` statement. A constructor can be provided as `__init__`; in general, method names that start and end with `__` define special methods, such as operators. As an example, the `__repr__` method of the `DataSet` is used for converting to a string for the `print` statement.

All non-static methods of a Python class must take the instance of the class as a first argument; this is commonly called `self`.

In Fig. B4, an example script is shown which creates a `DataSet` instance, creates some data ($y = x^2, x \in [0, 1]$) and makes a plot using plotting functionality from the pyalps package. We store the legend string and the axis labels for the final plot into

```
def subtract_spectrum(s1,s2,tolerance=1e-12):
    res = pyalps.DataSet()
    res.props = s1.props

    for i in range(len(s1.x)):
        remove = False
        for j in range(len(s2.x)):
            if abs(s1.x[i]-s2.x[j]) < tolerance and abs(s1.y[i]-s2.y[j]) < tolerance:
                remove = True
                break
        if not remove:
            res.x = np.append(res.x,s1.x[i])
            res.y = np.append(res.y,s1.y[i])

    return res
```

Figure B2. Example of a Python function from the pyalps package. The function takes two `DataSet` instances as input and returns a new `DataSet` that contains all (x,y) values that occur in the first but not in the second. The intended use is for plotting of spectra, where states that occur in several quantum number sectors should sometimes be shown only once.

```
class DataSet(ResultProperties):
  def __init__(self):
    ResultProperties.__init__(self)

    self.x = np.array([])
    self.y = np.array([])

  def __repr__(self):
    return "x=%s\ny=%s\nprops=%s" % (self.x, self.y, self.props)
```

Figure B3. Simple example of a Python class from the pyalps package.

```
import pyalps
from pyalps.plot import plot
import numpy as np
import matplotlib.pyplot as plt

ds = pyalps.DataSet()
ds.x = np.linspace(0,1,10)
ds.y = ds.x**2
ds.props['xlabel'] = '$\gamma$'
ds.props['ylabel'] = '$\gamma^2$'
ds.props['label'] = 'Example legend'

plot([ds])
plt.legend()
plt.show()
```

Figure B4. Plotting a simple function with pyalps.

Name	*Description*
`Boost_LIBRARY_PATH`	Path to the Boost source tree. If Boost is not available as binary, this has to be set by the user when first running `cmake`.
`CMAKE_C_COMPILER`	`C` compiler. This is determined from the system path or environment variable `CC`.
`CMAKE_CXX_COMPILER`	`C++` compiler. This is determined from the system path or environment variable `CXX`.
`PYTHON_INTERPRETER`	Path of the Python interpreter that `pyalps` should be built for. If not set, a default be determined or Python is disabled.

Table C1. List of CMake variables that have to be provided when first running `cmake`. These cannot be changed afterwards.

the `props` dict of the `DataSet` instance. Note that the plotting function from pyalps is passed a list with one `DataSet` – this function, like most other pyalps functions, operates directly on lists of `DataSet`s in order to assist the user in dealing with larger sets of data.

Appendix C. ALPS Installation with CMake

Appendix C.1. Prerequisites

The following tools and libraries are required to build ALPS:

- The CMake build system [42] of version 2.8.0 or newer.
- The BLAS [78] and LAPACK libraries [79]. Ideally optimized versions for the target architecture should be used instead of the generic netlib versions.
- The Boost C++ libraries version 1.43.0 or later (Boost 1.45.0 is included in one version of the source tarball) [49]. Boost does not have to be installed; instead, the ALPS installation process can build the required Boost libraries if necessary.
- The HDF5 library version 1.8 [35].
- A standard complying C++ compiler. ALPS has been tested with gcc versions 4.2, 4.3 and 4.4 as well as MSVC 9, IBM xlC++ 11.1, and Intel's icpc 10 and 11.

To build optional parts of ALPS it is recommended to install in addition:

- Python version 2.5 or 2.6 [50].
- The NumPy [58], SciPy [59], and matplotlib [52] Python packages.
- The VisTrails scientific workflow and provenance management system [39] and all its dependencies.
- A Fortran 90 compiler for the `tebd` code.

Name	*Description*
`CMAKE_INSTALL_PREFIX`	Installation prefix. Default is `/opt/alps`.
`VISTRAILS_APP_DIR`	Path to the directory where VisTrails is installed.
`ALPS_BUILD_APPLICATIONS`	Enable or disable build process for ALPS applications.
`ALPS_BUILD_EXAMPLES`	Enable or disable build process for ALPS examples.
`ALPS_BUILD_TESTS`	Enable or disable build process for ALPS tests.
`ALPS_BUILD_PYTHON`	Enable or disable build process for `pyalps`.
`HDF5_LIBRARIES`	Path of the HDF5 libraries.
`HDF5_INCLUDE_DIR`	Path to HDF5 header files.
`BLAS_LIBRARY`	Path of the BLAS library.
`LAPACK_LIBRARY`	Path of the LAPACK library.

Table C2. List of CMake variables that can be changed at any time. Some of these are mandatory, i.e., if ALPS is unable to determine a value automatically, an error will be generated.

Appendix C.2. The CMake build system

While we generally recommend the use of the binary installation packages whenever available, the source installation using the CMake build system may offer several advantages to experienced users:

- Specific compiler versions and optimization flags can be provided.
- The binary installers are tied to a specific version of Python, whereas the source installation can be built against the version of Python that the user prefers.
- Custom versions of external libraries such as the BLAS and LAPACK libraries can be provided.

The CMake build process is controlled by a set of variables describing the build environment, paths, and targets (libraries and programs) to be built. Most of these variables are automatically determined in the top-level file `CMakeLists.txt`. Each source directory also contains such a file with prescriptions for building certain targets given the global configuration variables. A major advantage of CMake over other build systems such as the `autotools` is that it allows the user easy access and modification of all variables via a graphical interface, the tool `ccmake` or by directly editing the file `CMakeCache.txt`.

With a few exceptions (which are listed below), all CMake variables can be changed at any point during the installation. CMake will be able to determine the effects of changing a variable and, if necessary, repeat the compilation of parts of ALPS given the new configuration. This gives the user the possibility to change aspects of the configuration without repeating the entire installation process.

Some of the most important CMake variables for the ALPS build system are listed in Tables C1 and C2. Note that library paths have to be given as absolute paths; if several libraries are required, e.g. for BLAS, the paths should be separated with semicolons.

An important point is linking against the correct versions of BLAS and LAPACK, since this may seriously affect the performance of some applications. ALPS will try to determine automatically which libraries should be used and will give optimized libraries like Intel's MKL precedence over standard libraries. Nevertheless, it is recommended to check whether this has been recognized correctly.

Appendix C.3. Installation steps

It is strongly recommended to perform the configuration and compilation of ALPS in a separate directory (*build directory*). Running any CMake commands in the source directory will likely cause problems in later stages. For concreteness, we will assume in the following that the ALPS source can be found in `/home/user/alps` and Boost sources can be found in `/home/user/boost_1_43_0`. For other libraries, we will assume that they are installed in standard system paths. All commands should be executed in the build directory, which initially must be empty.

The first step is to create an initial CMake configuration:

```
cmake -D Boost_ROOT_DIR:PATH=/home/user/boost_1_43_0 /home/user/alps
```

Additional variables can be passed with the `-D` flag. For example, if the HDF5 libraries are not found in a standard path, Python should not be used, and a non-standard compiler should be used, the following commands need to be executed:

```
export CC=/opt/local/bin/gcc-mp-4.4
export CXX=/opt/local/bin/g++-mp-4.4
cmake -D Boost_ROOT_DIR:PATH=/home/user/boost_1_43_0 \
-D HDF5_LIBRARIES=/home/user/HDF5/lib/libhdf5.so \
-D HDF5_INCLUDE_DIR=/home/user/HDF5/include \
-D ALPS_BUILD_PYTHON=OFF /home/user/alps
```

Please note that `cmake` should always be run from an empty directory. If an error occurs, please clear all files from the build directory before running `cmake` again. By default, CMake will generate a set of UNIX Makefiles. It is also possible to use other generators; for example, project files for XCode or KDevelop can be created.

In the next step, additional variables can be customized by either editing the file `CMakeCache.txt` directly, running the command `ccmake` or invoking the CMake GUI.

Now the standard procedure is to build, test, and install ALPS using

```
make
make test
make install
```

The VisTrails packages can also be installed from the CMake installation process. On UNIX or Linux platforms, it is sufficient to set the CMake variable `VISTRAILS_APP_DIR`. If, for example, the file `vistrails.py` from the VisTrails installation is found in the directory `/home/user/vistrails/vistrails/`, `VISTRAILS_APP_DIR` should be set to `/home/user/vistrails/`. On Mac OS X, a more advanced build type is needed since VisTrails delivers a specific version of Python. For instructions for this special case, we refer to our website.

```
<PARAMETERS>
  <PARAMETER name=”LATTICE”> square </PARAMETER>
  <PARAMETER name=”MODEL”>       spin </PARAMETER>
  <PARAMETER name=”L”>             10 </PARAMETER>
  <PARAMETER name=”T”>            0.5 </PARAMETER>
</PARAMETERS>
```

Figure D1. Excerpt from an XML file for simulation input parameters .

```
<SCALAR_AVERAGE name=”Susceptibility”>
  <MEAN>                         421.3 </MEAN>
  <ERROR converged=”yes”>         1.54 </ERROR>
  <VARIANCE>                  1.06e+05 </VARIANCE>
</SCALAR_AVERAGE>
```

Figure D2. Excerpt from an XML file for simulation results of the uniform susceptibility in a Monte Carlo simulation.

Appendix D. The ALPS XML schemas

XML is the format of choice for text-based ALPS files. Unlike simple formats, where the location of a number in the file specifies its meaning (e.g. the first number is system size, the second temperature), XML specifies the meaning of data through meta-information provided by markup with tags, as shown in figure D1 for input parameters and in figure D2 for simulation results. The meaning of these files is easy to decipher even years after the simulation, unlike many other formats. A resemblance to HTML is no chance, since HTML (XHTML) is indeed also an XML format. Instead of looking directly at the long (and sometimes ugly) output files in XML format, the XML files can be easily transformed to other formats using XSLT transformations[80] and viewed, e.g. directly as HTML in a web browser, or printed as plain text.

Besides XML schemas for parameter input and output of results we have developed XML schemas for the description of lattices and models. Examples are shown in figures D3 and D4. For detailed specification of the formats see our XML web page.[45]

Providing an input file (such as the one where an excerpt is shown in figure D1 together with lattice and model definitions in figures D3 and D4 to any of the ALPS applications will run that application on the given model (provided the application supports that type of models) and returns an output file containing data such as shown in figure D2.

Appendix D.1. Lattice definitions

Besides the ability to specify translation invariant lattices as shown in Fig. D3, starting in release 1.3 ALPS has included 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, or systems in spatially varying trapping potentials, such as optical

```
<LATTICEGRAPH name = "square">
  <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>
</LATTICEGRAPH>
```

Figure D3. The definition of a square lattice with one site (vertex) per unit cell and bonds (edges) only to nearest neighbors. After describing the dimension, extent and boundary conditions of the Bravais lattice in the `<FINITELATTICE>` element, the unit cell including the bonds in the lattice is defined.

```
<BASIS name="spin">
  <SITEBASIS>
    <QUANTUMNUMBER name="S" min="1/2" max="1/2"/>
    <QUANTUMNUMBER name="Sz" min="-S" max="S"/>
    <OPERATOR name="Splus" matrixelement="sqrt(S*(S+1)-Sz*(Sz+1))">
      <CHANGE quantumnumber="Sz" change="1"/>
    </OPERATOR>
    <OPERATOR name="Sminus" matrixelement="sqrt(S*(S+1)-Sz*(Sz-1))">
      <CHANGE quantumnumber="Sz" change="-1"/>
    </OPERATOR>
    <OPERATOR name="Sz" matrixelement="Sz"/>
  </SITEBASIS>
</BASIS>

<HAMILTONIAN name="spin">
  <BASIS ref="spin"/>
  <SITETERM> -h*Sz </SITETERM>
  <BONDTERM source="i" target="j">
    Jxy/2*(Splus(i)*Sminus(j) + Sminus(i)*Splus(j)) + Jz*Sz(i)*Sz(j)
  </BONDTERM>
</HAMILTONIAN>
```

Figure D4. The definition of a spin-1/2 XXZ spin Hamiltonian with one type of exchange coupling only: $H = -h\sum_i S_i^z + \sum_{\langle i,j\rangle} \left((J_{\mathrm{xy}}/2)(S_i^+ S_j^- + S_i^- S_j^+) + J_z S_i^z S_j^z\right)$. After describing the local basis for each site and operators acting on it, the Hamiltonian is defined.

lattices in harmonic traps. Inhomogeneities can be specified for vertices (sites) and edges (bonds), either for all (such as for all vertices in figure D5), or only for one type of vertex or edge.

One can also randomly deplete the lattice by removing 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. Please contact the authors if you need that feature. In the example in figure D5, the fraction of depleted

```
<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>
```

Figure D5. 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. The new feature shown here is the specification of an inhomogeneous lattice, allowing to specify different couplings on the sites (in this example), and the depletion of the vertices of the lattices.

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.

For more examples of lattices we refer the reader to the file `lattices.xml` included in ALPS that contains a number of commonly used lattices. A detailed discussion of the creation of lattice files is presented on the ALPS web page.

Appendix D.2. Model definitions

Figure D4 shows the simplest definition of an XXZ spin model with Hamiltonian

$$H = -h\sum_i S_i^z + \sum_{\langle i,j\rangle}\Big((J_{\rm xy}/2)(S_i^+S_j^- + S_i^-S_j^+) + J_z S_i^z S_j^z\Big) \tag{D.1}$$

Figure D6 shows the definition of the Hamiltonian of a bosonic Hubbard model in a harmonic trap

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

One feature 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.

```
<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>
```

Figure D6. The definition of a bosonic Hubbard Hamiltonian (D.2) in a harmonic trap. After describing the local basis for each site and operators acting on it, one can also 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, instead of writing all terms explicitly as in the example in Fig. D4. Another feature shown here is the use of the parameters x and y in the couplings to create spatially-dependent couplings when combined with an inhomogeneous lattice.

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 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 [81].

For more examples of models we refer the reader to the file `lattices.xml` included in ALPS that contains a number of commonly used models. A detailed discussion of the creation of model files is presented on the ALPS web page.

References

[1] Alet F, Dayal P, Grzesik A, Honecker A, Körner M, Läuchli A, Manmana S R, McCulloch I P, Michel F, Noack R M, Schmid G, Schollwöck U, Stöckli F, Todo S, Trebst S, Troyer M, Werner P and Wessel S 2005 *Journal of the Physical Society of Japan* **74S** 30–35

[2] Albuquerque A, Alet F, Corboz P *et al.* 2007 *Journal of Magnetism and Magnetic Materials* **310** 1187–1193

[3] Lanczos C 1950 *J. Res. Natl. Bur. Stand.* **49** 225

[4] White S R 1992 *Phys. Rev. Lett.* **69** 2863–2866

[5] Schollwöck U 2005 *Rev. Mod. Phys.* **77** 259–315

[6] Daley A J, Kollath C, Schollwöck U and Vidal G 2004 *Journal of Statistical Mechanics: Theory and Experiment* **2004** P04005

[7] White S R and Feiguin A E 2004 *Phys. Rev. Lett.* **93** 076401

[8] Vidal G 2003 *Phys. Rev. Lett.* **91** 147902

[9] Vidal G 2004 *Phys. Rev. Lett.* **93** 040502

[10] Verstraete F and Cirac J I 2004 *preprint cond-mat/0407066 (unpublished)*

[11] Murg V, Verstraete F and Cirac J I 2007 *Phys. Rev. A* **75** 033605

[12] Vidal G 2007 *Phys. Rev. Lett.* **99** 220405

[13] Swendsen R H and Wang J S 1987 *Phys. Rev. Lett.* **58** 86–88

[14] Wolff U 1989 *Phys. Rev. Lett.* **62** 361–364

[15] Evertz H G, Lana G and Marcu M 1993 *Phys. Rev. Lett.* **70** 875–879

[16] Prokof'ev N V, Svistunov B V and Tupitsyn I S 1998 *JETP Sov. Phys.* **87** 310

[17] Sandvik A W 1999 *Phys. Rev. B* **59** R14157–R14160

[18] Todo S and Kato K 2001 *Phys. Rev. Lett.* **87** 047203

[19] `http://wistaria.comp-phys.org/alps-looper/`

[20] Syljuåsen O F and Sandvik A W 2002 *Phys. Rev. E* **66** 046701

[21] Evertz H G 2003 *Advances in Physics* **52**(1) 1–66

[22] Alet F, Wessel S and Troyer M 2005 *Phys. Rev.E.* **71** 036706

[23] Wang F and Landau D P 2001 *Phys. Rev. Lett.* **86** 2050–2053

[24] Wang F and Landau D P 2001 *Phys. Rev. E* **64** 056101

[25] Troyer M, Wessel S and Alet F 2003 *Phys. Rev. Lett.* **90** 120201

[26] Trebst S, Huse D A and Troyer M 2004 *Phys. Rev. E* **70** 046701

[27] Katzgraber H, Trebst S, Huse D and Troyer M 2006 *Journal of Statistical Mechanics: Theory and Experiment* P03018

[28] Wessel S, Stoop N, Gull E, Trebst S and Troyer M 2007 *Journal of Statistical Mechanics: Theory and Experiment* P12005

[29] Rubtsov A N and Lichtenstein A I 2004 *JETP Letters* **80** 61–65

[30] Rubtsov A N, Savkin V V and Lichtenstein A I 2005 *Phys. Rev. B* **72** 035122

[31] Werner P, Comanac A, de' Medici L *et al.* 2006 *Phys. Rev. Lett.* **97** 076405

[32] Werner P and Millis A J 2006 *Phys. Rev. B* **74** 155107

[33] Gull E, Werner P, Parcollet O and Troyer M 2008 *EPL (Europhysics Letters)* **82** 57003

[34] `http://www.w3.org/XML/`

[35] `http://www.hdf5.org/`

[36] `http://alps.comp-phys.org/static/software//LICENSE.txt`

[37] `http://alps.comp-phys.org/static/software//LICENSE-applications.txt`

[38] `http://alps.comp-phys.org/`

[39] `http://www.vistrails.org/`

[40] `http://www.openmp.org/`

[41] `http://www.mpi-forum.org/`

[42] `http://www.cmake.org/`

[43] `http://www.macports.org/`

[44] `http://www.knoppix.net/`

[45] `http://xml.comp-phys.org/`

[46] Troyer M, Ammon B and Heeb E 1998 *Lecture Notes in Computer Science* **1505** 191

[47] Czarnecki K and Eisenecker U 2000 *Generative Programming* (Addison-Wesley)

[48] Siek J, Lee L Q and Lumsdaine A 2001 *The Boost Graph Library User Guide and Reference Manual* (Addison-Wesley)

[49] `http://www.boost.org/`

[50] `http://www.python.org/`

[51] Ambegaokar V and Troyer M 2010 *American Journal of Physics* **78** 150–157

[52] `http://matplotlib.sourceforge.net/`

[53] `http://plasma-gate.weizmann.ac.il/Grace/`

[54] `http://www.gnuplot.info/`

[55] `http://www.vtk.org/`

[56] Lutz M 2009 *Learning Python* (O'Reilly & Associates)

[57] Lutz M 2006 *Programming Python (Third Edition)* (O'Reilly & Associates)

[58] `http://numpy.scipy.org/`

[59] `http://www.scipy.org/`

[60] Sandvik A W and Kurkijärvi J 1991 *Phys. Rev. B* **43** 5950–5961

[61] `http://physics.mines.edu/downloads/software/tebd/`

[62] Georges A, Kotliar G, Krauth W and Rozenberg M J 1996 *Rev. Mod. Phys.* **68** 13

[63] Kotliar G, Savrasov S Y, Haule K *et al.* 2006 *Rev. Mod. Phys.* **78** 865

[64] Maier T, Jarrell M, Pruschke T and Hettler M H 2005 *Rev. Mod. Phys.* **77** 1027

[65] Hirsch J E and Fye R M 1986 *Phys. Rev. Lett.* **56** 2521–2524

[66] Gull E, Werner P, Fuchs S, Surer B, Pruschke T and Troyer M 2010 Continuous-time quantum monte carlo impurity solvers

[67] Silva C, Freire J and Callahan S 2007 *IEEE Computing in Science and Engineering* **9** 82

[68] Freire J, Koop D and Silva C 2008 *Computing in Science and Engineering* **10** 11

[69] Bavoil L, Callahan S, Crossno P, Freire J, Scheidegger C, Silva C and Vo H 2005 *Proceeding of IEEE Visualization* 18

[70] Lee E A and Parks T M 1995 *Proceedings of the IEEE* **83** 773–801

[71] Clifford B, Foster I, Hategan M, Stef-Praun T, Wilde M and Zhao Y 2007 *Concurrency and Computation: Practice and Experience*

[72] J Freire, C T Silva, S P Callahan, Santos E, Scheidegger C E and Vo H T 2006 Managing rapidly-evolving scientific workflows *International Provenance and Annotation Workshop (IPAW)* LNCS 4145 pp 10–18 invited paper

[73] Callahan S, J. Freire, Santos E, Scheidegger C, Silva C and Vo H 2006 Managing the Evolution of Dataflows with VisTrails *(Extended Abstract) IEEE Workshop on Workflow and Data Flow for Scientific Applications (SciFlow)*

[74] Scheidegger C E, Vo H T, Koop D, Freire J and Silva C T 2007 *IEEE Transactions on Visualization and Computer Graphics (Proceedings of Visualization)* **13** 1560–1567

[75] Bavoil L, Callahan S, Crossno P, J. Freire, Scheidegger C, Silva C and Vo H 2005 Vistrails: Enabling interactive multiple-view visualizations *Prof. of IEEE Visualization* pp 135–142

[76] Koop D, Santos E, Bauer B, Troyer M, Freire J and Silva C 2010 Bridging workflow and data provenance using strong links *Scientific and Statistical Database Management* (*Lecture Notes in Computer Science* vol 6187) ed Gertz M and Ludscher B (Springer Berlin / Heidelberg) pp 397–415

[77] Santos E, Lins L, Ahrens J, Freire J and Silva C 2009 *IEEE Transactions on Visualization and Computer Graphics* **15** 1539

[78] `http://www.netlib.org/blas/`

[79] `http://www.netlib.org/lapack/`

[80] `http://www.w3.org/TR/xslt/`

[81] Wessel S, Alet F, Troyer M and Batrouni G G 2004 *Phys. Rev. A* **70** 053615