Updated Core Libraries of the ALPS Project

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Abstract

The open source ALPS (Algorithms and Libraries for Physics Simulations) project provides a collection of physics libraries and applications, with a focus on simulations of lattice models and strongly correlated systems. The libraries provide a convenient set of well-documented and reusable components for developing condensed matter physics simulation code, and the applications strive to make commonly used and proven computational algorithms available to a non-expert community. In this paper we present an updated and refactored version of the core ALPS libraries geared at the computational physics software development community, rewritten with focus on documentation, ease of installation, and software maintainability.

PROGRAM SUMMARY

Program Title: ALPS Core libraries

Project homepage: <http://alpscore.org>

Catalogue identifier: –

Journal Reference: –

Operating system: Unix, Linux, OSX

Programming language: C++

Computers: any architecture with suitable compilers including PCs, clusters and supercomputers

RAM: Highly problem-dependent

Distribution format: GitHub, downloadable as zip

Licensing provisions: GNU General Public License

Classification: 6.5, 7.3, 20

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Preprint submitted to Computer Physics Communications

December 8, 2016

Keywords: Many-body physics, Strongly correlated systems, Monte Carlo, C++, High Performance Computing

External routines/libraries: CMake, MPI, Boost, HDF5.

Nature of problem: Need for modern, lightweight, tested and documented libraries covering the basic requirements of rapid development of efficient physics simulation codes, especially for modeling strongly correlated electron systems.

Solution method:

We present a C++ open source computational library that provides a convenient set of components for developing parallel physics simulation code. The library features a short development cycle and up-to-date user documentation.

Running time: Tests take of the order of several minutes; Otherwise highly problem dependent (from minutes to several days).

1. Introduction

The open source ALPS (Algorithms and Libraries for Physics Simulations) project [1, 2, 3] provides a collection of physics libraries and applications, especially suited for the simulation of lattice models and strongly correlated systems. The ALPS libraries provide well-documented, reusable components for developing condensed matter physics simulation code, while ALPS applications’ goal is to make commonly used and proven computational algorithms available to a non-expert community.

Computer codes based on the ALPS libraries have provided physical insights in many subfields of condensed matter. Highlights include nonequilibrium dynamics [4, 5], continuous-time quantum Monte Carlo [6, 7], LDA+DMFT materials simulations [8], simulations of quantum [9] and classical [10] spin, correlated boson [11] and fermion [12] models, as well as cuprate superconductivity [13].

In this paper we present an updated and refactored version of the main ALPS Libraries (here and thereafter referred to as “ALPS core libraries” or, as a whole, “the library”). The focus of the update is on providing a set of lightweight, thoroughly tested and documented libraries to code developers that implement generic algorithms and utilities for rapid development of efficient computational physics applications. Substantial portions of the code are significantly rewritten compared to the previous version of the ALPS Libraries, and special emphasis is placed on a short development cycle and up-to-date user documentation.

A snapshot of the code at the time of submission of this paper is available at the CPC program library. Later versions will be available from the main site, <http://alpscore.org>, together with in-depth user documentation, tutorials, and examples. Development versions of the library are available from the public Git repository at <https://github.com/ALPSCore/ALPSCore>. Several application codes are built on the core libraries and are distributed independently.

The remainder of this paper is organized as follows: In section 2 we introduce and motivate the library; in section 3, we provide an overview of the library components; in section 4, we list the software packages prerequisite for compiling and installing the library, as well as outline the installation procedure; in section 5, we describe the development and testing cycle of the library; in section 6 we specify the ALPS citation policy and license, and in sections 7 and 8 we summarize the paper and acknowledge our contributors. Additionally, Appendix A provides installation examples and Appendix B an

example of code using the library to program a two-dimensional Ising model simulation with single spin flip updates.

2. Motivation, target audience, philosophy

Our library is intended to be used by two communities: directly by computational physicists who develop their own computer codes, and indirectly by users who use applications based on the library. There are a number of challenges that such a scientific developer faces:

Framework/boilerplate code. A typical computational physics program (for example, a Monte Carlo simulation code) contains parts that have little to do with the scientific problem that the simulation strives to get insight into. Those parts form the necessary framework for running the simulation, and are responsible for various auxiliary tasks such as reading the parameters of the simulation or saving intermediate and final results. Auxiliary ‘boilerplate’ code is often imported with little or no changes from application to application. As writing the auxiliary code is secondary to solving the scientific problem at hand, it is therefore given less attention. However, the auxiliary code is not necessarily trivial and redeveloping it from scratch results in unnecessary duplication of effort and reduced code quality.

Code reuse problem. For the same reasons, physics code often lacks modularization: parts of the code are not properly separated by well-defined interfaces, and the scientific code is buried deep inside the boilerplate/framework. The resulting lack of interoperability hinders the exchange of code with other research groups and results in further unnecessary duplication of effort.

Process management. As codes grow, they become progressively more difficult to manage and document. The lack of modularity and documentation makes it hard for researchers outside the primary developers group to contribute to the project. A possibility of unintentional disruption of code functionality by introducing changes effectively discourages implementing new features.

High performance computing requirements. Although programming in a high-level language (such as `Python`) may help in solving the framework/boilerplate code problem, the use of a high-level language is often problematic. Computational physics algorithms are complex, and the computational kernels implementing them are resource-demanding and in most of the cases must make use of multi-node and multi-core capabilities of contemporary HPC (High Performance Computing) hardware. The high-performance requirements necessitate implementation of the kernels in a lower-level language, such as `C++`, and utilizing `MPI` and `OpenMP` parallel programming techniques. The task of including high-performance parallelized kernels into high-level language framework, although technically feasible, is far from being trivial.

The purpose of the ALPS core libraries is to reduce the user’s time and effort to develop and test complex scientific applications. This project addresses the above-mentioned challenges by providing reusable and widely-used, high-performance, well-

documented software building blocks with open architecture. To facilitate reuse, the library utilizes high level of abstraction without compromising performance. To encourage reuse and contributions, the library strives to maintain current user-level and developer-level documentation, easy installation procedure, as well as a short development cycle with rapid bugfixes and frequent releases. The manageability requirements are addressed via documented code, modular structure, and extensive testing. The project is open to contributions in the form of bug reports, feature requests, and code.

3. Some of the key library components

In this section, we provide a brief overview of the purpose and functionality of some of the key components comprising the ALPS core libraries. Additional information is available online and as part of the `Doxygen` code documentation. It should be noted that the components maintain minimal interdependence, and using a component in a program does not bring in other components, unless they are required dependencies, in which case they will be used automatically.

Building a parallel Monte Carlo simulation. A generic Monte Carlo simulation can be easily assembled from the classes provided by *Monte Carlo Scheduler* component. The programmer needs to define only the problem-specific methods that are called at each Monte Carlo step, such as methods to update the configuration of the Monte Carlo chain and to collect the measured data. The simulation is parallelized implicitly, using one MPI process per chain. [Appendix B](#) contains an example of a Monte Carlo simulation using these Scheduler classes.

Computing observable averages, errors, correlation times, and cross-correlation. To collect Monte Carlo simulation data and to estimate and propagate Monte Carlo errors of potentially correlated data, the *Accumulators* library component is to be used, especially in cases where correlations in time or cross-correlations between different variables exist. The Accumulator objects support arithmetic operations and elementary mathematical functions, e.g. division of one observable by another or the multiplication of two observables. The non-linear error propagation through these operations is also supported.

Several Accumulator objects provide different trade-offs between memory consumption, overhead time, and functionality. In order of decreasing memory and measurement requirements they are:

1. **FullBinningAccumulator**: provides access to data autocorrelation length, autocorrelation-corrected error bars, and proper error propagation in non-linear functions using Jackknife [14] resampling technique.
2. **LogBinningAccumulator**: provides access to data autocorrelation estimates and autocorrelation-corrected error bars.
3. **NoBinningAccumulator**: estimates the error bars of the data without regard to autocorrelation.
4. **MeanAccumulator**: maintains only the mean value of the data (no error bars or autocorrelation length).

A typical use of accumulators in a Monte Carlo simulation is demonstrated in [Appendix B](#).

Storing, restoring, and checkpointing simulation results. To store the results of a simulation in a cross-platform format for subsequent analysis, one can use the *Archive* component. The component provides convenient interface to saving and loading of common C++ data structures (primitive types, complex numbers, STL vectors and maps), as well as of objects of user-defined classes HDF5 [15], which is the universally supported and machine independent data format. Use of the Archive component for application checkpointing is illustrated in [Appendix B](#).

Reading command-line arguments and parameter files. Input parameters to a simulation can be passed via a combination of a parameter file and command line arguments. The *Parameters* library component is responsible for parsing the files and the command line, and providing access to the data in the form of an associative array (akin to C++ map or Python dictionary). The parameter files use the standard “*.ini” format, a plain text format with a line-based syntax containing key = value pairs, optionally divided into sections. The use of the Parameters component is illustrated in [Appendix B](#).

Working with Green’s functions. The *Green’s Functions* component provides a type-safe interface to manipulate objects representing bosonic or fermionic many-body Green’s functions, self-energies, susceptibilities, polarization functions, and similar objects. From a programmer’s perspective, these objects are multidimensional arrays of floating-point or complex numbers, defined over a set of meshes and addressable by a tuple of indices, each belonging to a grid. Currently, Matsubara (imaginary frequency), imaginary time, power, momentum space, real space, and arbitrary index meshes are supported.

These many-body objects often need to be supplemented with analytic tail information encapsulating the high frequency / small time moments of the Green’s functions, so that high precision Fourier transforms, density evaluations, or energy evaluations can be performed. The Green’s function library component provides this functionality in addition to saving to and loading from binary HDF5 files. An example illustrating the use of the Green’s function classes is given in [Appendix C](#).

4. Prerequisites and Installation

To build the ALPS core libraries, any recent C++ compiler can be used; the libraries are tested with GCC [16] 4.2 and above, Intel [17] C++ 10.0 and above, and Clang [18] 3.2 and above. The library follows the C++03 standard [19] to facilitate the portability to a wide range of programming environments, including HPC clusters with older compilers. The library depends on the following external packages:

- The CMake build system [20] of version 2.8.12 and above.
- The Boost C++ libraries [21] of version 1.54.0 and above. Compiled libraries are only needed from the program option, serialization, and file system libraries.
- The HDF5 library [15] version 1.8 and above.

To make use of (optional) parallel capabilities, an MPI implementation supporting standard 2.1 [22] and above is required. Generating the developer’s documentation requires Doxygen [23] along with its dependencies.

The installation of the ALPS core libraries follows the standard procedure for any CMake-based package. The first step is to download the ALPS core libraries source code; the recommended way is to download the latest ALPS core libraries release from <https://github.com/ALPSCore/ALPSCore/releases>. Assuming that all above-mentioned prerequisite software is installed, the installation consists of unpacking the release archive and running CMake from a temporary build directory, as outlined in the shell session example below (the \$ sign designates a shell prompt):

```
$ tar -xzf ALPSCore-0.5.4.tar.gz
$ mkdir build
$ cd build
$ export ALPSCore_DIR=$HOME/software/ALPSCore
$ cmake -DCMAKE_INSTALL_PREFIX=$ALPSCore_DIR \
        -DCMAKE_BUILD_TYPE=Release \
        ../ALPSCore-0.5.4
$ make
$ make test
$ make install
```

The command at line 1 unpacks the release archive (version 0.5.4 in this example); at line 4 the destination install directory of the ALPS core libraries is set (\$HOME/software/ALPSCore in this example).

The ALPS core libraries come with an extensive set of tests; it is strongly recommended to run the tests (via `make test`) to verify the correctness of the build, as it is done at line 9 in the example above.

The installation procedure is outlined in more details in [Appendix A](#); also, the file `common/build/build.jenkins.sh` in the library release source tree contains a build and installation script that can be further consulted for various build options.

On Mac OS X operating system, the ALPS core libraries package can be downloaded and installed from the MacPorts [24] or HomeBrew [25] repositories, using commands `port install alpscore` or `brew tap homebrew/science && brew install alpscore`, respectively.

5. Development and Test Cycle

The ALPS core libraries development emphasizes a short development cycle and frequent releases of operational code, along with user-level and programmer-level documentation. The techniques we employ to achieve these goals are discussed below.

5.1. Distributed version control and collaborative development

In accordance with modern software practices, all changes introduced in the course of development of ALPS core libraries are tracked using a distributed version control system, Git [26]. The version control system preserves the history of changes in every source file in its database (the Git repository), associating each change (a “commit”) with its originator, and allows the author to comment on each set of changes. The version control system allows one to create independent lines of code development (branches), with subsequent optional merging of those lines.

The master version of the repository with ALPS core libraries, which is publicly available for downloading, is hosted on the GitHub [27] hosting service. The distributed nature of Git allows any developer to work independently on his or her own copy (“clone”) of the repository, and then request to merge his or her clone into this publicly-visible

repository (submit a “pull request”); after reviewing the code changes that the developer made, the request is granted by one of the members of the core development team.

In addition to the repository, GitHub provides an issue tracker. Any registered GitHub user is able to submit a question, a bug report or a feature request via the tracking system. The developer team is notified that a new issue is open and then triages the issue, marking it according to its severity (for example, “bug”, “enhancement”, “question”); assigns a developer to be responsible for it; and associates a code development “milestone” with it. The issue can be further commented on by other users and developers, creating a thread of conversation. Once the issue is resolved or otherwise addressed, it is marked as “closed”.

GitHub also provides hosting space for Wiki pages, which the project uses for user-level documentation and tutorials. The Wiki documentation contains direct links to repository code, and thus simplifies keeping the code samples up to date. The ALPS core libraries project encourages collaboration and feedback from the user community by opening issues, submitting pull requests, and contributing to the Wiki documentation pages.

5.2. Test-driven development and continuous integration

Test-driven development (TDD) is a software development process that emphasizes creating a test for a feature prior to implementing it. Among the advantages of TDD are increased test coverage (because every new feature has a corresponding test), higher confidence in test validity (because the test is ensured to fail on unimplemented feature) and improved code quality [28]. We follow the TDD process in the development of the ALPS core libraries, whenever practical.

Typically, each test verifies the behavior of a single function or object method in isolation from other methods of the same class; this approach is known as “unit testing”. However, many components of ALPS core libraries depend on functionality provided by other components (for example, Monte Carlo scheduler uses Accumulators and Parameters). In this way, a unit test of an object method provided by a component tests the coordinated working of the component’s dependencies, and can be considered a form of integration test. It should also be noted that only publicly accessible (rather than private) methods are invoked in testing. In our development process, a unit tests is also a form of documentation, demonstrating both the correct way to call a method and the interface specification.

In order to avoid maintenance problems associated with merging several branches of development and possible breaking of code functionality, the ALPS core libraries development adopted the Continuous Integration [29] practice. Continuous Integration prescribes frequent merging of the code into the main repository and running tests (in our case, the unit/integration test suite) to make sure that the code functions as expected. To build the code and run the test suite we utilize the Jenkins Continuous Integration tool [30]. In order to conduct unit and integration testing of the ALPS core libraries on wider range of operating environments, we make use of a cloud-based service (provided by CloudBees [31]). When a developer merges his or her series of commits into the central repository, an automated upload to the cloud-based service occurs, followed by building of the library and running the test suites in different environments, under different operating systems (Linux and Mac OS X) and using various versions of compilers and libraries. The test results are immediately available for developers to analyze and correct any errors.

The same build process also generates developer-level documentation from documenting comments embedded in the code.

Once all outstanding issues are resolved, new features are implemented or existing ones are improved, and the test suites are passed in all supported environments, a developer requests GitHub to generate a release. By virtue of the Continuous Integration process, the code in repository at that stage is ensured to be free of known issues; therefore, the release is essentially a compressed archive of the snapshot of the repository, ready to be installed and deployed. When the state of the repository is marked as a release, a request is automatically sent to the Zenodo [32] service to download and archive the release in Zenodo's searchable database; Zenodo also generates a citable DOI code associated with the release. The complete development and test cycle of the ALPS core libraries project, discussed above, is illustrated by Figure 1.

Figure 1: Development cycle of ALPS core libraries. Developer's commit to public GitHub repository causes automatic rebuild on CloudBees service via Jenkins. Releases are automatically published on Zenodo.

6. License and citation policy

The GitHub version of ALPS core libraries is licensed under the GNU General Public License version 2 (GPL v. 2) [33] or later; for compatibility reasons with the journal the version released here is licensed under GPL v. 3. The older ALPS license under which previous versions of the code were licensed [3] has been retired. We kindly request that the present paper be cited, along with any relevant original physics or algorithmic paper, in any published work utilizing an application code that uses this library.

7. Summary

We have presented an updated and repackaged version of the core ALPS libraries, a lightweight C++ library, designed to facilitate rapid development of computational physics applications, and have described its main features. The collaborative, test-driven development process utilizing the continuous integration approach has been also described.

8. Acknowledgments

Work on the ALPS library project is supported by the Simons collaboration on the many-electron problem. Aspects of the library are supported by NSF DMR-1606348 and DOE ER 46932.

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URL <http://www.gnu.org/licenses/gpl.html>

Appendix A. Detailed installation procedure

In the following discussion we assume that all prerequisite software (section 4) is installed, and the ALPS core libraries release (here, release 0.5.4) is downloaded into the current directory as `ALPSCore-0.5.4.tar.gz`. Also, we assume that the libraries are to be installed in `ALPSCore` subdirectory of the current user's home directory. The commands are given assuming `bash` as a user shell.

The first step is to unpack the release archive and set the desired install directory:

```
$ tar -xzf ALPSCore-0.5.4.tar.gz 1
$ export ALPSCore_DIR=$HOME/software/ALPSCore 2
```

The next step is to perform the build of the library (note that the build should not be performed in the source directory):

```
$ mkdir build 3
$ cd build 4
$ cmake ../ALPSCore-0.5.4 -DCMAKE_INSTALL_PREFIX=$ALPSCore_DIR \ 5
    -DCMAKE_BUILD_TYPE=Release 6
```

The `cmake` command at lines 5 and 6 accepts additional arguments in the format `-Dvariable=value`. A number of relevant CMake variables is listed in Table A.1. The installation process is also affected by environment variables, some of which are listed in Table A.2; the CMake variables take precedence over the environment variables. The build and installation script `common/build/build.jenkins.sh` in the ALPS core libraries release source tree provides an example of using some of the build options.

Appendix B. Example: 2D Ising model

Appendix B.1. Problem statement

This program implements a single-spin update Metropolis Monte Carlo algorithm for computing properties of a well-known two-dimensional Ising model. The system under consideration is a square lattice of spins $\{s_i = \pm 1\}$; the periodic boundary conditions are imposed, with a unit cell of size $L \times L$, containing $N = L^2$ spins. The energy per spin is given by

$$E = -\frac{1}{N} \sum_{(i,j)} s_i s_j \quad (\text{B.1})$$

where (i, j) runs over all nearest-neighbor pairs in the unit cell. The magnetization per spin is given by

$$M = \frac{1}{N} \sum_i s_i \quad (\text{B.2})$$

where i runs over all $N = L^2$ spins in the unit cell.

The properties of interest are thermal averages of energy $\langle E \rangle$, magnetization $\langle M \rangle$, absolute value of magnetization $\langle |M| \rangle$ and Binder cumulant:

$$U = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2} \quad (\text{B.3})$$

computed at temperature T (inverse temperature $\beta = 1/T$) expressed in energy units.

Appendix B.2. Build process

The build of the example program is controlled by the `CMakeLists.txt` file given by the Listing 1.

Listing 1: CMakeLists.txt file

```

cmake_minimum_required(VERSION 2.8.12)
project(ising2_mc CXX)

add_executable(${PROJECT_NAME} main.cpp ising.cpp)
add_executable(${PROJECT_NAME}_mpi main_mpi.cpp ising.cpp)

# Request the ALPSCore package (with all components)
# The ALPSCore package must be installed in some
# standard place (like /usr/local),
# or somewhere in your PATH.
# Otherwise, point ALPSCore_DIR environment variable
# to the ALPSCore installation tree.
find_package(ALPSCore REQUIRED)

# Use ALPSCore_LIBRARIES variable to link to ALPSCore
target_link_libraries(${PROJECT_NAME} ${ALPSCore_LIBRARIES})
target_link_libraries(${PROJECT_NAME}_mpi ${ALPSCore_LIBRARIES})

```

Variable	Default value	Comment
CMAKE_CXX_COMPILER	(system default)	Path to C++ compiler executable.*
CMAKE_INSTALL_PREFIX	/usr/local	library target install directory.
CMAKE_BUILD_TYPE		Specifies build type; set to Release to maximize performance.
BOOST_ROOT		Boost install directory. Set if CMake fails to find Boost.
Boost_NO_SYSTEM_PATHS	false	Set to true to disable search in default system directories, if the wrong version of Boost is found.
Boost_NO_BOOST_CMAKE	false	Set to true to disable search for Boost CMake file, if the wrong version of Boost is found.
Documentation	ON	Build developer's documentation.
ENABLE_MPI	ON	Enable MPI build (set to OFF to disable).
Testing	ON	Build unit tests (recommended).
ALPS_BUILD_TYPE	dynamic	Can be dynamic or static : build libraries as dynamic ("shared") or static libraries, respectively.* (<i>Since ALPSCore 0.5.5</i>)
<i>For ALPSCore version 0.5.4 and older:</i>		
ALPS_BUILD_SHARED	ON	Build shared ALPS core libraries.* Mutually exclusive with ALPS_BUILD_STATIC=ON.
ALPS_BUILD_STATIC	OFF	Build static ALPS core libraries.* Mutually exclusive with ALPS_BUILD_SHARED=ON.

*Note: For the change of this variable to take effect, remove your build directory and redo the build.

Table A.1: CMake arguments relevant to building of ALPS core libraries.

Variable	Comment
CXX	Path to C++ compiler executable.*
BOOST_ROOT	Boost install directory. Set if CMake fails to find Boost.
HDF5_ROOT	HDF5 install directory. Set if CMake fails to find HDF5.

*Note: For the change of this variable to take effect, remove your build directory and redo the build.

Table A.2: Environment variables arguments relevant to building of ALPS core libraries.

Lines 4 and 5 specify the source files that constitute the sequential and parallel versions of the program, respectively. Line 13 requests the ALPS core libraries (ALPSCore) package that must be installed as described in section [Appendix A](#); the installation location must be in one of standard system directories such as `/usr/local`, in one of the directories listed in the `PATH` environment variable, or in a directory pointed to by `ALPSCore_DIR` environment variable. Lines 16 and 17 specify that the sequential and parallel versions of the program use libraries provided by the ALPSCore package.

Assuming that the ALPS core libraries are installed as described above, the example code is located in `/path/to/source` directory, and the project is to be built in `/path/to/build` directory, the following commands will build the project (the `$` sign designates a shell prompt):

```
$ cd /path/to/build
$ cmake /path/to/source
$ make
```

Two executable files, `ising2_mc` for the sequential version, and `ising2_mc_mpi` for the parallel version, will be generated in the current directory.

Appendix B.3. Monte Carlo simulation class

The simulation class encapsulates the details of building a Markov chain, sampling observables (in this case, the energy, magnetization, *etc.*), and keeping track of the progress of the calculation. Our simulation class `ising_sim` is declared in Listing 2, line 11.

Listing 2: `ising.hpp` header file: Declares interface of the simulation class

```
#pragma once

#include <alps/mc/mcbase.hpp>
#include "storage_type.hpp"

// Simulation class for 2D Ising model (square lattice).
// Extends alps::mcbase, the base class of all Monte Carlo simulations.
// Defines its state, calculation functions (update/measure) and
// serialization functions (save/load)
class ising_sim : public alps::mcbase {
    // The internal state of our simulation
private:
    int length; // the same in both dimensions
    int sweeps;
    int thermalization_sweeps;
    int total_sweeps;
    double beta;
    storage_type spins;
    double current_energy;
    double current_magnetization;

public:
    ising_sim(parameters_type const & parms, std::size_t seed_offset = 0);
    static void define_parameters(parameters_type & parameters);
    virtual void update();
    virtual void measure();
    virtual double fraction_completed() const;

    using alps::mcbase::save;
    using alps::mcbase::load;
```

```

36         virtual void save(alps::hdf5::archive & ar) const;
37         virtual void load(alps::hdf5::archive & ar);
38     };

```

The simulation class is required to inherit from `alps::mcbase`, and it must define the following virtual methods with the corresponding semantics:

- `void update()` (line 30): Attempt a step in the phase space, accept or reject it;
- `void measure()` (line 31): Compute and accumulate observables;
- `double fraction_completed() const` (line 32): report the fraction of the computation that is completed.

Also, a static method `void define_parameters()` (line 28) should be provided that declares (“defines”) the input parameters pertinent to the simulation (see section 3).

Listing 2 also declares a number of implementation-specific private data members (lines 14–23) holding the internal state of the Markov chain. The `include` statement in line 4 refers to the header file containing implementation details: storage of spins in a two-dimensional array; for the sake of completeness, the implementations of the corresponding class is briefly discussed in subsection [Appendix B.7](#).

The implementation of the simulation class is provided by `ising.cpp` file.¹ Lines 5–21 in the implementation file (Listing 3) define the input parameters that are relevant to the simulation: size of the unit cell, number of thermalization Monte Carlo steps, total number of steps, and the simulation temperature. Note that each parameter name has an associated type, and parameters “sweeps” and “thermalization” are given default values (0 and 10000, respectively); the other two parameters (“length” and “temperature”) do not have default values and are required to be provided by the user. In addition, a number of standard parameters used in every Monte Carlo simulation is defined by the base class; the corresponding static method is called at line 12. Line 15 defines a number of parameters common for many simulations.

Listing 3: `ising.cpp` file: Implementation of the simulation class: Parameter definition

```

1  #include "ising.hpp"
2  #include <alps/params/convenience_params.hpp>
3
4  // Defines the parameters for the ising simulation
5  void ising_sim::define_parameters(parameters_type & parameters) {
6      // If the parameters are restored, they are already defined
7      if (parameters.is_restored()) {
8          return;
9      }
10
11      // Adds the parameters of the base class
12      alps::mcbase::define_parameters(parameters);
13      // Adds the convenience parameters (for save/load)
14      // followed by the ising specific parameters
15      alps::define_convenience_parameters(parameters)
16          .description("2D ising simulation")
17          .define<int>("length", "size of the periodic box")
18          .define<int>("sweeps", 0, "maximum number of sweeps (0 means
19              indefinite)")

```

¹The code presented here and in the following discussion is written with the focus on simplicity and clarity rather than efficiency.

```

6         .define<int>("thermalization", 10000, "number of sweeps for      19
7             thermalization")
8         .define<double>("temperature", "temperature of the system");    20
9     }                                                                    21

```

The object constructor (Listing 4) initializes the internal state of the simulation in lines 27–56. Additionally, lines 59–66 allocate named accumulators for the observables to be collected during the simulation.

Listing 4: `ising.cpp` file: Implementation of the simulation class: Constructor

```

15 // Creates a new simulation.                                           23
16 // We always need the parameters and the seed as we need to pass it to  24
17 // the alps::mcbase constructor. We also initialize our internal state,  25
18 // mainly using values from the parameters.                            26
19 ising_sim::ising_sim(parameters_type const & parms, std::size_t seed_offset  27
20 )
21 {
22     : alps::mcbase(parms, seed_offset)                                28
23     , length(parameters["length"])                                    29
24     , sweeps(0)                                                       30
25     , thermalization_sweeps(int(parameters["thermalization"]))        31
26     , total_sweeps(parameters["sweeps"])                              32
27     , beta(1. / parameters["temperature"].as<double>())              33
28     , spins(length, length)                                           34
29     , current_energy(0)                                               35
30     , current_magnetization(0)                                        36
31 }
32
33 // Initializes the spins                                              37
34 for(int i=0; i<length; ++i) {                                       38
35     for (int j=0; j<length; ++j) {                                   39
36         spins(i,j) = (random() < 0.5 ? 1 : -1);                     40
37     }                                                                41
38 }                                                                    42
39
40 // Calculates initial magnetization and energy                       43
41 for (int i=0; i<length; ++i) {                                       44
42     for (int j=0; j<length; ++j) {                                   45
43         current_magnetization += spins(i,j);                         46
44         int i_next=(i+1)%length;                                     47
45         int j_next=(j+1)%length;                                     48
46         current_energy += -(spins(i,j)*spins(i,j_next)+              49
47                             spins(i,j)*spins(i_next,j));           50
48     }                                                                51
49 }                                                                    52
50
51 // Adds the measurements                                             53
52 measurements                                                         54
53 << alps::accumulators::FullBinningAccumulator<double>("Energy")    55
54 << alps::accumulators::FullBinningAccumulator<double>("            56
55     Magnetization")
56 << alps::accumulators::FullBinningAccumulator<double>("            57
57     AbsMagnetization")
58 << alps::accumulators::FullBinningAccumulator<double>("            58
59     Magnetization^2")
60 << alps::accumulators::FullBinningAccumulator<double>("            59
61     Magnetization^4")
62 ;                                                                    60
63 }                                                                    61
64                                                                    62
65                                                                    63
66                                                                    64
67                                                                    65
68                                                                    66

```

Implementation of the Monte Carlo step and the acceptance/rejection logic by the method `update()` (Listing 5, lines 70–97) is straightforward.

Listing 5: `ising.cpp` file: Implementation of the simulation class: Update method

```

54 // Performs the calculation at each MC step;                          68
55
56
57
58
59
60
61
62
63
64
65

```

```

6 // decides if the step is accepted.
7 void ising_sim::update() {
8     using std::exp;
9     typedef unsigned int uint;
10    // Choose a spin to flip:
11    uint i = uint(length * random());
12    uint j = uint(length * random());
13    // Find neighbors indices, with wrap over box boundaries:
14    uint i1 = (i+1) % length; // right
15    uint i2 = (i-1+length) % length; // left
16    uint j1 = (j+1) % length; // up
17    uint j2 = (j-1+length) % length; // down
18    // Energy difference:
19    double delta=2.*spins(i,j)*
20        (spins(i1,j)+ // right
21         spins(i2,j)+ // left
22         spins(i,j1)+ // up
23         spins(i,j2)); // down
24
25    // Step acceptance:
26    if (delta<=0. || random() < exp(-beta*delta)) {
27        // update energy:
28        current_energy += delta;
29        // update magnetization:
30        current_magnetization -= 2*spins(i,j);
31        // flip the spin
32        spins(i,j) = -spins(i,j);
33    }
34 }

```

The `measure()` method (Listing 6, lines 100–113) adds the observables of interest to the corresponding named accumulators (lines 108–112).

Listing 6: `ising.cpp` file: Implementation of the simulation class: Measurement method

```

32 // Collects the measurements at each MC step.
33 void ising_sim::measure() {
34     ++sweeps;
35     if (sweeps<thermalization_sweeps) return;
36     const double n=length*length; // number of sites
37     double tmag = current_magnetization / n; // magnetization
38
39     // Accumulate the data (per site)
40     measurements["Energy"] << (current_energy / n);
41     measurements["Magnetization"] << tmag;
42     measurements["AbsMagnetization"] << fabs(tmag);
43     measurements["Magnetization^2"] << tmag*tmag;
44     measurements["Magnetization^4"] << tmag*tmag*tmag*tmag;
45 }

```

The `fraction_completed()` method (Listing 7, lines 116–122) returns a `double` value. This value indicates whether the simulation ran the intended number of steps: the simulation stops when the value reaches 1.0. The termination criteria are discussed in more details in [Appendix B.6](#).

Listing 7: `ising.cpp` file: Implementation of the simulation class: Report completed fraction

```

50 // Returns a number between 0.0 and 1.0 with the completion percentage
51 double ising_sim::fraction_completed() const {
52     double f=0;
53     if (total_sweeps>0 && sweeps >= thermalization_sweeps) {
54         f=(sweeps-thermalization_sweeps)/double(total_sweeps);
55     }
56     return f;
57 }

```


The implementation file `ising.cpp` also contains definitions of methods that are necessary for checkpointing the simulation, as discussed in [Appendix B.5](#).

Appendix B.4. Main program

We first describe the flow of the sequential implementation, postponing the discussion of the parallelization till subsection [Appendix B.6](#). The sequential main program (`main.cpp`) is shown in Listings 8 and 9; a few essential points are discussed in this and the following subsections.

Line 19 of Listing 8 constructs a parameter object from the command line arguments: an optional name of a parameter file followed by an optional set of parameters in the form of “`--key=value`”. The parameter values that are set in the command line override the values set in the parameter file. The parameter names and types must be declared before use, which is done at line 20 by a call to a static method `define_parameters()` of the simulation class. Lines 22–25 check if the user requested help or missed a required argument. The simulation is created at line 28, with the parameters passed to the constructor. Line 41 starts the simulation.

Listing 8: `main.cpp` file: Main program, sequential version: Starting the simulation

```

1  #include "ising.hpp"
2  #include <iostream>
3  #include <alps/accumulators.hpp>
4  #include <alps/mc/api.hpp>
5  #include <alps/mc/mcbase.hpp>
6  #include <alps/mc/stop_callback.hpp>
7
8  int main(int argc, char* argv[])
9  {
10     // Define the type for the simulation
11     typedef ising_sim my_sim_type;
12
13     try {
14
15         // Creates the parameters for the simulation
16         // If an hdf5 file is supplied, reads the parameters there
17         std::cout << "Initializing parameters..." << std::endl;
18
19         alps::params parameters(argc, (const char**)argv);
20         my_sim_type::define_parameters(parameters);
21
22         if (parameters.help_requested(std::cout) ||
23             parameters.has_missing(std::cout)) {
24             return 1;
25         }
26
27         std::cout << "Creating simulation" << std::endl;
28         my_sim_type sim(parameters);
29
30         // If needed, restore the last checkpoint
31         std::string checkpoint_file = parameters["checkpoint"].as<std::string>();
32
33         if (parameters.is_restored()) {
34             std::cout << "Restoring checkpoint from " << checkpoint_file
35                 << std::endl;
36             sim.load(checkpoint_file);
37         }
38
39         // Run the simulation
40         std::cout << "Running simulation" << std::endl;
41         sim.run(alps::stop_callback(size_t(parameters["timelimit"])));

```

The results of the simulation (the accumulated observables) are retrieved at line 48 (Listing 9). The `results` object is streamed to standard output which prints out all the accumulated results. Individual observables can be accessed by name, as shown by lines 56–62. The observable is represented by an object of type `result_wrapper` from namespace `alps::accumulators`; each object has associated mean value, error bar and autocorrelation length. It is possible to conduct arithmetic operations and compute functions of the `result_wrapper` objects, as illustrated by line 65 computing Binder cumulant (per equation (B.3)); the error bars of the operands are propagated when an expression is evaluated. Finally, at lines 73–76 the simulation parameters and the results are saved to a file in HDF5 format; the name of the file is passed via input parameter “outputfile” which is defined earlier in the simulation implementation file `ising.cpp` (by the call at line 15 of Listing 3).

Listing 9: `main.cpp` file: Main program, sequential version: Collecting the results

```

42 // Checkpoint the simulation
43 std::cout << "Checkpointing simulation to " << checkpoint_file
44 << std::endl;
45 sim.save(checkpoint_file);
46
47 alps::results_type<my_sim_type>::type results = alps::
48 collect_results(sim);
49
50 // Print results
51 {
52     using alps::accumulators::result_wrapper;
53     std::cout << "All measured results:" << std::endl;
54     std::cout << results << std::endl;
55
56     std::cout << "Simulation ran for "
57 << results["Energy"].count()
58 << " steps." << std::endl;
59
60     // Assign individual results to variables.
61     const result_wrapper& mag4=results["Magnetization^4"];
62     const result_wrapper& mag2=results["Magnetization^2"];
63
64     // Derived result:
65     const result_wrapper& binder_cumulant=1-mag4/(3*mag2*mag2);
66     std::cout << "Binder cumulant: " << binder_cumulant
67 << " Relative error: "
68 << fabs(binder_cumulant.error<double>())/
69 binder_cumulant.mean<double>())
70 << std::endl;
71
72     // Saving to the output file
73     std::string output_file = parameters["outputfile"];
74     alps::hdf5::archive ar(boost::filesystem::path(output_file), "w
75 ");
76     ar["/parameters"] << parameters;
77     ar["/simulation/results"] << results;
78
79     return 0;
80 } catch (const std::runtime_error& exc) {
81     std::cout << "Exception caught: " << exc.what() << std::endl;
82     return 2;
83 } catch (...) {
84     std::cout << "Unknown exception caught." << std::endl;
85     return 2;
86 }

```

Appendix B.5. Checkpointing

Listing 10 focuses on the part of the main program that is relevant for checkpointing. Once the simulation is completed, at line 46 of the file `main.cpp` the state of the simulation object is saved to a file via a call to method `save()`, which takes the file name as an argument. If the first argument to the program is a name of a file in HDF5 format, the parameter object constructor restores the parameters (including their associated types and values) from the file (the values of individual parameters still can be overridden from the command line). Lines 33–37 check if the parameters are read from an HDF5-formatted file, and, if so, the simulation object is restored from the checkpoint file via call to method `load()`, which, like `save()`, takes the file name as an argument. Both `save()` and `load()` methods are provided by the base simulation class `alps::mcbase`.

Listing 10: `main.cpp` file: Main program, sequential version: Checkpointing

```
// If needed, restore the last checkpoint
std::string checkpoint_file = parameters["checkpoint"].as<std::
string>();

if (parameters.is_restored()) {
    std::cout << "Restoring checkpoint from " << checkpoint_file
    << std::endl;
    sim.load(checkpoint_file);
}

// Run the simulation
std::cout << "Running simulation" << std::endl;
sim.run(alps::stop_callback(size_t(parameters["timelimit"])));

// Checkpoint the simulation
std::cout << "Checkpointing simulation to " << checkpoint_file
    << std::endl;
sim.save(checkpoint_file);
```

However, to support checkpointing, user's simulation class `ising_sim` must provide `save()` and `load()` methods that take a reference to an object of `alps::hdf5::archive` type. In our example code, those methods are defined in the simulation implementation file `ising.cpp` (Listing 11), lines 125–136 (`save()`) and 139–155 (`load()`).

Listing 11: `ising.cpp` file: Implementation of the simulation class: Checkpointing

```
// Saves the state to the hdf5 file
void ising_sim::save(alps::hdf5::archive & ar) const {
    // Most of the save logic is already implemented in the base class
    alps::mcbase::save(ar);

    // We just need to add our own internal state
    ar["checkpoint/spins"] << spins;
    ar["checkpoint/sweeps"] << sweeps;
    ar["checkpoint/current_energy"] << current_energy;
    ar["checkpoint/current_magnetization"] << current_magnetization;

    // The rest of the internal state is saved as part of the parameters
}

// Loads the state from the hdf5 file
void ising_sim::load(alps::hdf5::archive & ar) {
    // Most of the load logic is already implemented in the base class
    alps::mcbase::load(ar);

    // Restore the internal state that came from parameters
    length = parameters["length"];
    thermalization_sweeps = parameters["thermalization"];
```

```

146 // Note: 'total_sweeps' is not restored here!
147 beta = 1. / parameters["temperature"].as<double>();
148
149 // Restore the rest of the state from the hdf5 file
150 ar["checkpoint/spins"] >> spins;
151 ar["checkpoint/sweeps"] >> sweeps;
152 ar["checkpoint/current_energy"] >> current_energy;
153 ar["checkpoint/current_magnetization"] >> current_magnetization;
154
155 }

```

Most of the logic is implemented in the corresponding methods of the parent class; the `save()` method saves only the part of the internal state that changed since construction of the object (lines 130–133), and the `load()` method both restores those variables (lines 151–154) and re-initializes the rest of the internal state from the parameters (lines 144–147).

For all basic types and many common C++ aggregate types (such as STL vectors, vectors of STL vectors, and others) the saving to and loading from an HDF5 archive are supported via a simple streaming operators `<<` and `>>`, as shown in lines 131–133 and 152–154. However, to support archiving of the `spins` object (lines 130 and 151) which is of the user-defined type `storage_type`, similar methods `save()` and `load()` must be defined in the corresponding class, as discussed in subsection [Appendix B.7](#).

Appendix B.6. Scheduling and parallelization

Normally, the sequential simulation terminates once it has run to completion, as determined by the value returned by the method `fraction_completed()` of the simulation class. However, the method `run()` of the simulation base class `alps::mcbase` accepts a function object argument: the “stop callback”. This callback is called repeatedly during the simulation and is expected to return a boolean value: `false` if the simulation can continue, `true` if the simulation must be stopped. The library provides convenience function objects of class `alps::stop_callback`. The class constructor takes the maximum simulation time (in seconds) as an argument; the constructed function object returns `true` if the maximum simulation time has elapsed since the moment of the object construction, or if the program is interrupted by a signal. The use of the `alps::stop_callback` class facilitates a “graceful” termination of the simulation in the case of timeout or interruption by a user.

In order to parallelize the simulation, only minimal changes are required in the main program, and no changes are needed in the simulation class. The parallel version of the main program is given by Listing 12.

Listing 12: `main_mpi.cpp` file: Main program, parallel version

```

1 #include "ising.hpp"
2 #include <iostream>
3 #include <alps/accumulators.hpp>
4 #include <alps/mc/api.hpp>
5 #include <alps/mc/mcbase.hpp>
6 #include <alps/mc/stop_callback.hpp>
7 #include <alps/mc/mpiadapter.hpp>
8
9 int main(int argc, char* argv[])
10 {
11     // Define the type for the simulation
12     typedef alps::mcmpiadapter<ising_sim> my_sim_type;
13

```

```

14 // Initialize the MPI environment, and obtain the WORLD communicator
15 alps::mpi::environment env(argc, argv);
16 alps::mpi::communicator comm;
17 const int rank=comm.rank();
18 const bool is_master=(rank==0);
19
20 try {
21     // Creates the parameters for the simulation
22     // If an hdf5 file is supplied, reads the parameters there
23     if (is_master) std::cout << "Initializing parameters..." << std:::
24         endl;
25
26     // This constructor broadcasts to all processes
27     alps::params parameters(argc, (const char**)argv, comm);
28     my_sim_type::define_parameters(parameters);
29
30     if (parameters.help_requested(std::cout) ||
31         parameters.has_missing(std::cout)) {
32         return 1;
33     }
34
35     std::cout << "Creating simulation on rank " << rank << std::endl;
36     my_sim_type sim(parameters, comm);
37
38     // If needed, restore the last checkpoint
39     std::string checkpoint_file = parameters["checkpoint"].as<std:::
40         string>();
41     if (!is_master) checkpoint_file+="."+boost::lexical_cast<std:::
42         string>(rank);
43
44     if (parameters.is_restored()) {
45         std::cout << "Restoring checkpoint from " << checkpoint_file
46             << " on rank " << rank << std::endl;
47         sim.load(checkpoint_file);
48     }
49
50     // Run the simulation
51     std::cout << "Running simulation on rank " << rank << std::endl;
52     sim.run(alps::stop_callback(size_t(parameters["timelimit"])));
53
54     // Checkpoint the simulation
55     std::cout << "Checkpointing simulation to " << checkpoint_file
56         << " on rank " << rank << std::endl;
57     sim.save(checkpoint_file);
58
59     alps::results_type<my_sim_type>::type results = alps::
60         collect_results(sim);
61
62     // Print results
63     if (is_master) {
64         using alps::accumulators::result_wrapper;
65         std::cout << "All measured results:" << std::endl;
66         std::cout << results << std::endl;
67
68         std::cout << "Simulation ran for "
69             << results["Energy"].count()
70             << " steps." << std::endl;
71
72         // Assign individual results to variables.
73         const result_wrapper& mag4=results["Magnetization^4"];
74         const result_wrapper& mag2=results["Magnetization^2"];
75
76         // Derived result:
77         const result_wrapper& binder_cumulant=1-mag4/(3*mag2*mag2);
78         std::cout << "Binder cumulant: " << binder_cumulant
79             << " Relative error: "
80             << fabs(binder_cumulant.error<double>())/
81                 binder_cumulant.mean<double>()
82             << std::endl;
83
84         // Saving to the output file
85         std::string output_file = parameters["outputfile"];
86         alps::hdf5::archive ar(boost::filesystem::path(output_file), "w

```

```

1
2
3
4
5
6         ");
7         ar["/parameters"] << parameters;
8         ar["/simulation/results"] << results;
9     }
10    return 0;
11    } catch (const std::runtime_error& exc) {
12        std::cout << "Exception caught: " << exc.what() << std::endl;
13        env.abort(2);
14        return 2;
15    } catch (...) {
16        std::cout << "Unknown exception caught." << std::endl;
17        env.abort(2);
18        return 2;
19    }
20 }

```

At line 12, the `alps::mcmpiadapter` template parametrized by the user's simulation class (in our example, `ising_sim`) is used as the simulation class. The MPI environment is initialized and an MPI communicator is obtained (lines 15–17). The parameters object is created using a special broadcasting constructor (line 26) that takes the MPI communicator as an argument. Likewise, the parallel simulation constructor takes the communicator as its argument at line 35 (and ensures that each of the parallel simulation clones has its random number generator initialized with a different seed). Line 39 accounts for the fact that each of the parallel MPI processes now has its own checkpoint file. The results are seamlessly retrieved at line 56 from all parallel processes; the master process is responsible for processing and printing the results, as checked at line 59. Finally, if an exception is raised during the simulation, all MPI processes are aborted (lines 89 and 93).

In the case of the parallel execution, the simulation is considered completed if the *sum* of values returned by `fraction_completed()` methods of all parallel instances of the simulation class reaches 1, or if a termination requested by the “stop callback” in any of the instances. However, to reduce unnecessary interprocess communications, the completeness condition is checked at varying time intervals, within the limits specified by input parameters “Tmin” and “Tmax”. It should be noted that the check of the completeness condition is a collective operation: this must be taken into account if the user code invokes MPI collective operations on its own. It is therefore recommended, to avoid a possibility of a deadlock, that any collective operation initiated inside `update()` or `measure()` method should be completed before the method returns.

Appendix B.7. Other implementation details

The 2D-array storage type to keep values of spins is presented in Listing 13. For the sake of clarity and simplicity, spins are stored as a vector of integer vectors. Note that the class also defines method for saving to and loading from an HDF5 file (lines 27–33).

Listing 13: `storage_type.hpp` header file: Implementation of a 2D-array

```

1  #pragma once
2
3  #include <vector>
4  #include <alps/hdf5.hpp>
5
6  // Storage class for 2D spin array.
7  // Implemented as vector of vectors for simplicity.
8  class storage_type {
9  private:
10     std::vector< std::vector<int> > data_;
11 public:

```

```

1
2
3
4
5
6 // Constructor
7 storage_type(int nrows, int ncols):
8     data_(nrows, std::vector<int>(ncols))
9 {}
10
11 // Read access
12 int operator()(int i, int j) const {
13     return data_[i][j];
14 }
15 // Read/Write access
16 int& operator()(int i, int j) {
17     return data_[i][j];
18 }
19 // Custom save
20 void save(alps::hdf5::archive& ar) const {
21     ar["2Darray"] << data_;
22 }
23 // Custom load
24 void load(alps::hdf5::archive& ar) {
25     ar["2Darray"] >> data_;
26 }
27 };
28
29
30
31
32
33
34

```

Appendix B.8. Sample run and results

For the sake of the example, some parameters for the run are provided via a parameter file (see Listing 14).

Listing 14: ising2_mc.ini parameter file

```

29 # Size of the box:
30 length=4
31 # Time limit
32 timelimit = 3600
33
34
35
36
37
38
39
40
41
42
43
44
45
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61
62
63
64
65

```

Running of the parallel version on 2 CPU cores with example input parameters produces the following:

```

37 $ mpiexec -n 2 ./ising2_mc_mpi ising2_mc.ini --temperature=5 --timelimit=60
38 Initializing parameters...
39 Creating simulation on rank 0
40 Running simulation on rank 0
41 Creating simulation on rank 1
42 Running simulation on rank 1
43 Checkpointing simulation to ising2_mc.clone.h5.1 on rank 1
44 Checkpointing simulation to ising2_mc.clone.h5 on rank 0
45 All measured results:
46 AbsMagnetization: Mean +/-error (tau): 0.342837 +/-0.000101316(12.6489)
47 Energy: Mean +/-error (tau): -0.456241 +/-0.000168541(10.7416)
48 Magnetization: Mean +/-error (tau): -0.000150723 +/-0.000275311(31.4836)
49 Magnetization^2: Mean +/-error (tau): 0.175277 +/-9.02575e-05(13.7491)
50 Magnetization^4: Mean +/-error (tau): 0.0730068 +/-6.40981e-05(12.6128)
51
52 Simulation ran for 147922660 steps.
53 Binder cumulant: Mean +/-error (tau): 0.207852 +/-0.000218572(12.6128)
54 Relative error: 0.00105158
55
56
57
58
59
60
61
62
63
64
65

```

and creates files ising2_mc.out.h5, ising2_mc.clone.h5 and ising2_mc.clone.h5.1 in the current directory.

The program was run on a set of pre-generated parameter files with varying temperature and system size; the standard output was parsed and formatted for plotting by a simple script. The results are presented in figure B.2.

Figure B.2: The results of the 2D Ising model calculation implemented using ALPS core libraries, with periodic box of sizes $L = 4$, $L = 8$ and $L = 16$. The quantities plotted against the temperature T are: (a) Mean energy $\langle E \rangle$ per spin; (b) Absolute value of magnetization $\langle |M| \rangle$ per spin; (c) Autocorrelation length, per spin (logarithmic scale) of magnetization M ; (d) Binder cumulant for magnetization distribution.

Appendix C. Example: Green's Functions interface

Listing 15 illustrates working with Green's functions.

Listing 15: Working with Green's Function demo

```
#include <alps/gf/gf.hpp>
#include <alps/gf/tail.hpp>
#include <boost/array.hpp>

namespace g=alps::gf;

// Generates points for momentum mesh
g::momentum_index_mesh::container_type generate_momentum_mesh();

void Demo() {
    const int nspins=2;
    const int nfreq=10;
    const double beta=5;

    // Construct the meshes:
    g::matsubara_positive_mesh m_mesh(beta, nfreq);
    g::momentum_index_mesh k_mesh(generate_momentum_mesh());
    g::index_mesh s_mesh(nspins);

    // construct a GF using a pre-defined convenience type
    g::omega_k_sigma_gf gf(m_mesh, k_mesh, s_mesh);
    // initialize a GF to all-zeros
    gf.initialize();
}
```



```

1
2
3
4
5
6 // Make indices:
7 g::matsubara_index omega;
8 omega=4;
9 g::momentum_index ii(2);
10 g::index sigma(0);
11
12 // Assign a GF element:
13 gf(omega,ii,sigma)=std::complex<double>(3,4);
14
15 // Density matrix as a double-valued GF
16 // on momentum and integer-index space:
17 typedef
18     g::two_index_gf<double, g::momentum_index_mesh, g::index_mesh>
19     density_matrix_type;
20
21 // Construct the object:
22 density_matrix_type denmat=density_matrix_type(k_mesh,s_mesh);
23
24 // prepare diagonal matrix
25 const double U=3.0;
26 denmat.initialize();
27 // loop over first mesh index:
28 for (g::momentum_index i=g::momentum_index(0);
29      i<denmat.mesh1().extent(); ++i) {
30     denmat(i,g::index(0))=0.5*U;
31     denmat(i,g::index(1))=0.5*U;
32 }
33
34 // construct a tailed GF using predefined convenience type:
35 g::omega_k_sigma_gf_with_tail gft(gf);
36 gft.set_tail(0, denmat); // set the tail
37
38 density_matrix_type gftail=gft.tail(0); // retrieve the tail
39
40 // access the tailed GF element
41 std::complex<double> x=gft(omega,ii,sigma);
42 }
43
44 /// Generates 4 2-D points k_1,...,k_4 where each point k=(k_x,k_y)
45 g::momentum_index_mesh::container_type generate_momentum_mesh() {
46     const boost::array<int,2> dimensions={{4,2}};
47     g::momentum_index_mesh::container_type mesh_points(dimensions);
48     mesh_points[0][0]=0; mesh_points[0][1]=0; // (0,0)
49     mesh_points[1][0]=M_PI; mesh_points[1][1]=M_PI; // (pi,pi)
50     mesh_points[2][0]=M_PI; mesh_points[2][1]=0; // (pi,0)
51     mesh_points[3][0]=0; mesh_points[3][1]=M_PI; // (0,pi)
52     return mesh_points;
53 }

```

At lines 17–19 three meshes are constructed: a Matsubara mesh, a mesh in momentum space, and a general index mesh used here for the spin variable. Then, at line 22 a predefined convenience type is used to create a Green’s function defined on a Cartesian product of these three meshes. An element of the Green’s function can only be addressed by a tuple of 3 indices each belonging to a corresponding mesh, as shown in the listing: lines 27–30 define the indices and assign values to them, and line 33 accesses the Green’s function element.

Lines 37–39 define a Green’s function type `density_matrix_type` explicitly as a floating-point (C++ `double`) valued function defined on a Cartesian product of two meshes: the momentum mesh and the spin mesh. Here, a density matrix represented as an object of this type. The loop over the momentum index (lines 48–52) illustrates the use of inequality and increment operators on a mesh index to set values of the density matrix.

At line 55 a Green's function with a known tail is created from a regular Green's function. The tail encapsulates a high frequency expansion of a Green's function as:

$$G(i\omega_n, x \dots) = c_0(x \dots) + \frac{c_1(x \dots)}{i\omega_n} + \frac{c_2(x \dots)}{(i\omega_n)^2} + \dots \quad (\text{C.1})$$

where ω_n is Matsubara frequency, $c_j(j = 0, \dots)$ are tail coefficients of j -th order, and $x \dots$ represent all other arguments of a multi-dimensional Green's function. Note that the tail coefficients in this representation are themselves functions defined over $(x \dots)$.

At line 56 of the listing [15](#), the density matrix `denmat` is set as the 0-th order tail coefficient.

Finally, lines 65–73 define the function used to generate the momentum space mesh: the mesh contains 4 points, and each point (k_x, k_y) lies in a 2-dimensional momentum space.