The ALPS Project

Open Source Software for Strongly Correlated Systems

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for the ALPS collaboration

The ALPS collaboration

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The ALPS project

Algorithms and **L**ibraries for **P**hysics **S**imulations

- **open source** data formats, libraries and simulation codes for quantum lattice models

- download codes from website **http://alps.comp-phys.org**

Main Page

Welcome to the ALPS project.

The **ALPS project** (**A**lgorithms and **L**ibraries for **P**hysics **S**imulations) is an open source effort aiming at providing high-end simulation codes for strongly correlated quantum mechanical systems as well as C++ libraries for simplifying the development of such code. ALPS strives to increase software reuse in the physics community.

These Wiki pages serve as an interactive medium to develop current and future ALPS related web pages, first and foremost, the creation of a novel set of tutorial web pages, see the tutorial pages. To contribute to this Wiki you will need to have an account allowing you to edit the content of the Wiki pages.

Setup and Installation

Useful information **how to install** the alps libraries and applications on workstations and clusters.

Running an application

How to run and restart applications on workstations and clusters.

Tutorials

We are generating a series of new tutorial web pages that shall **facilitate the usage of the ALPS software** to solve physics problems.

Community

Check back regularly to read the **latest news** and information on the **people** contributing to the Wiki.

User Forum

Go here to **discuss** the ALPS libraries and applications with the community of developers. This is the place to address any questions you encounter while using any codes of the ALPS project.

et cetera

Go here to **find papers** on the ALPS project, **talks** from the first user workshop and a list of papers citing the ALPS project.

You can find the old static ALPS HTML pages here: [1]

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This page was last modified 10:58, 11 July 2006. This page has been accessed 1,463 times.

Open "http://alps.comp-phys.org/wiki/index.php/Main_Page" in a new tab

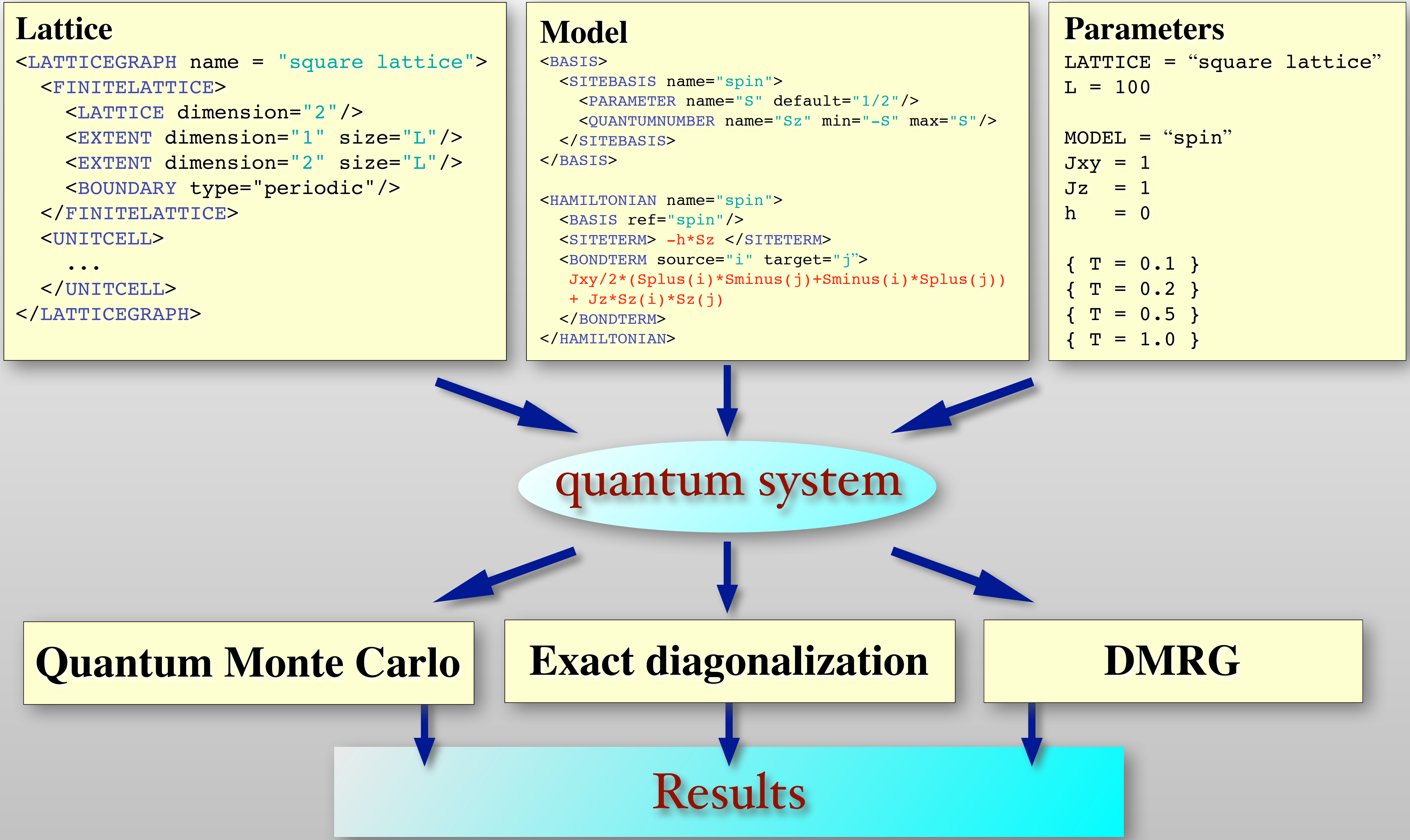
The tiers of ALPS

1. **Standard data formats and interfaces** to facilitate
    - exchange, archiving and querying of simulation results
    - exchange of simulation and analysis tools
2. **Libraries**
    - to support standard data formats and interfaces
    - to ease building of parallel simulation programs
3. **Evaluation tools**
    - to ease data evaluation and plotting
    - to record provenance information
4. **Applications**
    - to be used also by non-experts
    - implement modern algorithms for a large class of models

The ALPSCore spin-off

- ALPS comes as a large integrated package
- can be used also by non-experts
    - binary installers for Windows, Mac OS, ...
    - integration into VisTrails graphical workflow system
- demand from developers for more lightweight library modules for most commonly used functionalities
    - to be used in their own simulation codes
    - fewer dependencies, easier installation on high-performance systems
    - well tested
- this is what ALPSCore aims for: alpscore.org
    - actively developed by UMichigan team

Simulations with ALPS



Lattice

```
<LATTICEGRAPH name = "square lattice">
  <FINITELATTICE>
    <LATTICE dimension="2"/>
    <EXTENT dimension="1" size="L"/>
    <EXTENT dimension="2" size="L"/>
    <BOUNDARY type="periodic"/>
  </FINITELATTICE>
  <UNITCELL>
    ...
  </UNITCELL>
</LATTICEGRAPH>
```

Model

```
<BASIS>
  <SITEBASIS name="spin">
    <PARAMETER name="S" default="1/2"/>
    <QUANTUMNUMBER name="Sz" min="-S" max="S"/>
  </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>
```

Parameters

```
LATTICE = “square lattice”
L = 100

MODEL = “spin”
Jxy = 1
Jz  = 1
h   = 0

{ T = 0.1 }
{ T = 0.2 }
{ T = 0.5 }
{ T = 1.0 }
```

quantum system

Quantum Monte Carlo

Exact diagonalization

DMRG

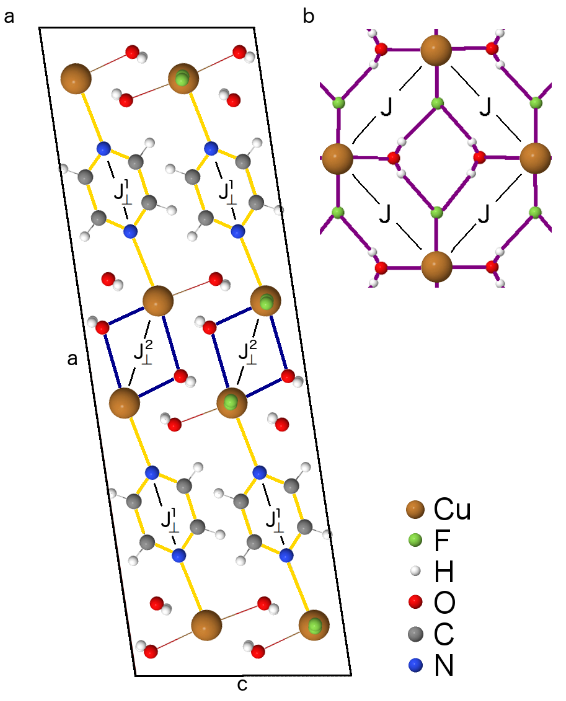
Results

Current applications

- **Classical Monte Carlo**
  - local and cluster updates for classical spin systems, M. Troyer
- **Quantum Monte Carlo**
  - stochastic series expansions (SSE), S. Isakov
  - loop code for spin systems, S. Todo
  - continuous time worm code, S. Trebst, M. Troyer
  - extended ensemble simulations, S. Wessel, N. Stoop
- **Exact diagonalization**
  - full and sparse, A. Honecker, A. Läuchli, M. Troyer
- **DMRG and variants** A. Feiguin, L. D. Carr, M. L. Wall, B. Bauer, M. Dolfi
- **DMFT:** E. Gull, B. Surer, P. Werner

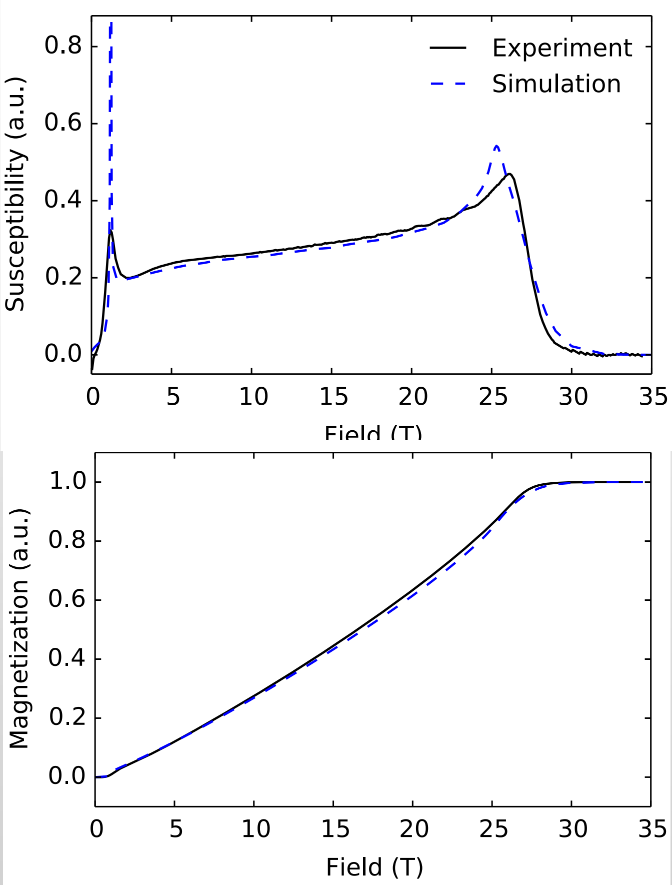
Heisenberg antiferromagnet

- metal-organic system
  - $(CuF_2(H_2O)_2)_2$-pyrazine
- measured in high magnetic fields
- model: spin-1/2 on square lattice
  - antiferromagnetic coupling in layer
  - weak interlayer coupling
- simulate with quantum Monte Carlo
  - SSE, see lecture by Roger Melko tomorrow



Heisenberg antiferromagnet

- define lattice unit cell in XML file
  - if not already among the standard lattices
- prepare, run and evaluate simulations
  - e.g. with Python script:
  - define model parameters
  - run simulations
  - load results
  - calculate derived observables, e.g. susceptibility
  - plot results
- for details see Björn Wehinger’s poster



Tutorials

- ALPS comes with an extensive set of tutorials
  http://alps.comp-phys.org/mediawiki/index.php/ALPS_2_Tutorials:Overview
  - for classical and Quantum Monte Carlo,
  - exact diagonalization,
  - DMRG,
  - DMFT,
  - TEBD
- see MC-01(a) for an example of binning analysis in action