強相関電子系/スピン系の汎用シミュレータ: ALPS

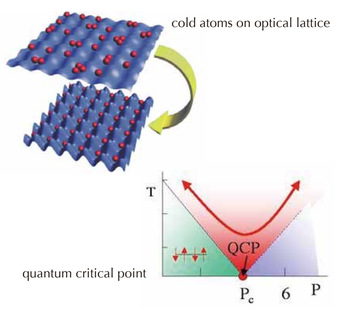
藤堂眞治 (東大院理/物性研/ALPS Collaboration)

Why quantum lattice models?

QLM: quantum spin models, bosonic Hubbard models, etc

- Effects of strong correlations in multi-degree-of-freedom systems
  - various types of long-range order
  - quantum disordered phase (quantum liquids, spin gap phases)
  - phase transitions and critical phenomena
    - quantum critical point
- Powerful simulation algorithms
  - quantum Monte Carlo methods
    exact diagonalization, DMRG, etc

- Universality
  - depends on few parameters: dimensionality, symmetry of order parameter, etc



QMC challenges for spin/bosonic lattice models

- Criticality with large (logarithmic) corrections to scaling (Kosterlitz-Thouless transition, phase transition in upper critical dimension, etc)
- Supersolid: co-existence of diagonal and off-diagonal order in frustrated spin/bosonic lattice models
- Deconfined criticality: direct continuous quantum phase transition between long-range ordered phase with incompatible symmetries (or weak 1st order phase transition?)
- Long-range interacting system (magnetic dipole, RKKY, etc): change of effective spatial dimension, exotic boundary effects, etc
- Strongly anisotropic systems (layered magnets, etc)
- ...

⇒ large-scale parallel simulations on the K Computer

The ALPS/looper Library

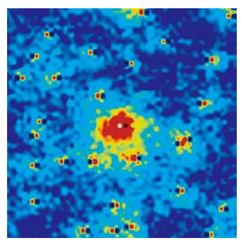
Multi-Cluster Quantum Monte Carlo Library

Generic QMC Library
- successor of Looper 2 (Fortran 90)

Based on ALPS framework
- implemented in C++
- ALPS/Lattice Library
- ALPS/Model Library, etc

Models
- generic XXZ Hamiltonians
- generic lattices
- any spin size S

Method
- path-integral and SSE representations
- multi-cluster loop algorithm
- hybrid (MPI + OpenMP) parallelization for K Computer



http://wistaria.comp-phys.org/alps-looper/

The ALPS Project

Algorithms and Libraries for Physics Simulations

Open source libraries and simulation code for strongly correlated quantum systems
- quamtum Monte Carlo
- exact diagonalization
- DMRG
- DMFT, etc

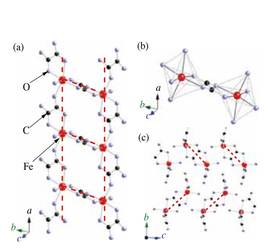
Motivation
- established algorithms
- increased demand for reliable simulations from theorists and experimentalists

The status quo
- individual codes
- model-specific implementations
- growing complexity of methods
- outputs in non-portable formats

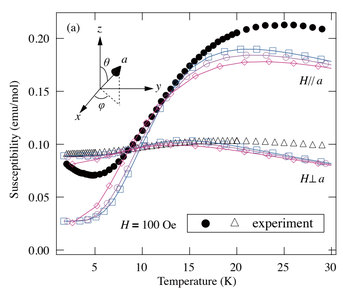
ALPS
- community codes
- generic implementations
- common libraries simplify code development
- common file formats

Spin Ladder Material $Na_2Fe_2(C_2O_4)_3(H_2O)_2$

- Fe2+ ions in octahedral crystal field
  → effective S=1 spins at low T
- Fitting experimental data by QMC results for several theoretical models (chain, ladder, dimer, etc)

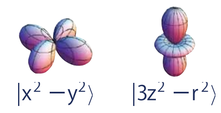


Yamaguchi et al (2009)

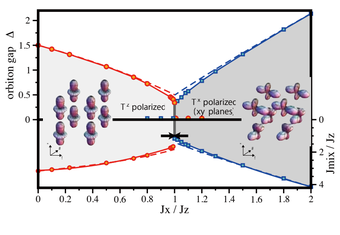


Orbital Ordering in e_g Orbital Systems

- Mott insulators with partially filled d-shells
- Non-tivial interplay of charge, spin, and orbital degrees of freedom
- Effective Hamiltonian for orbital degrees of freedom (120 degree model)



$$H_{120} = -\sum_{i,\gamma=x,y} \frac{1}{4}\left[J_z T_i^z T_{i+\gamma}^z + 3J_x T_i^x T_{i+\gamma}^x \pm \sqrt{3} J_{mix}\left(T_i^z T_{i+\gamma}^x + T_i^x T_{i+\gamma}^z\right)\right] - \sum_i J_z T_i^z T_{i+z}$$



van Rynbach et al (2010)

The ALPS Framework

tools	XML manipulation Python binding GUI	
applications	MC QMC ED DMRG DMFT	
domain-specific libraries	lattice model observables scheduler	
numerics	random ublas (Boost library)	iterative eigenvalue solver
generic C++	graph	serialization XML/XSLT
C / Fortran	BLAS LAPACK MPI HDF5	

A Simulation with ALPS

Parameter File

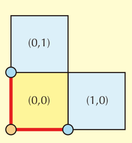
```
LATTICE = "square lattice"
MODEL   = "spin"
L       = 16
Jxy     = 1
Jz      = 2
SWEEPS  = 10000
THERMALIZATION = 1000

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

parameter2xml tool

Lattice XML File
square lattice

```
<LATTICES>
  <LATTICE name="square lattice" dimension="2">
    <PARAMETER name="a" default="1"/>
    <BASIS><VECTOR>a 0</VECTOR><VECTOR>0 a</VECTOR></BASIS>
  </LATTICE>
  <UNITCELL name="simple2d" dimension="2">
    <VERTEX/>
    <EDGE>
      <SOURCE vertex="1" offset="0 0"/>
      <TARGET vertex="1" offset="1 0"/>
    </EDGE>
    <EDGE>
      <SOURCE vertex="1" offset="0 0"/>
      <TARGET vertex="1" offset="0 1"/>
    </EDGE>
  </UNITCELL>
  <LATTICEGRAPH name="square lattice">
    <FINITELATTICE>
      <LATTICE ref="square lattice"/>
      <EXTENT dimension="1" size="L"/>
      <EXTENT dimension="2" size="L"/>
      <BOUNDARY type="periodic"/>
    </FINITELATTICE>
    <UNITCELL ref="simple2d"/>
  </LATTICEGRAPH>
</LATTICES>
```



Model XML File

$$H = J \sum_{<ij>} [S_i^z S_j^z + (S_i^+ S_j^- + S_i^- S_j^+)/2] - h \sum_i S_i^z$$

```
<MODELS>
  <BASIS name="spin">
    <SITEBASIS name="spin">
      <PARAMETER name="local_S" default="1/2"/>
      <QUANTUMNUMBER name="S" min="local_S" max="local_S"/>
      <QUANTUMNUMBER name="Sz" min="-S" max="S"/>
      <OPERATOR name="Sz" matrixelement="Sz"/>
      <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>
    </SITEBASIS>
  </BASIS>
  <HAMILTONIAN name="spin">
    <PARAMETER name="J" default="1"/>
    <PARAMETER name="h" default="0"/>
    <BASIS ref="spin"/>
    <SITETERM>
      -h * Sz(i)
    </SITETERM>
    <BONDTERM source="i" target="j">
      J * (Sz(i)*Sz(j) + (Splus(i)*Sminus(j)+Sminus(i)*Splus(j)))/2
    </BONDTERM>
  </HAMILTONIAN>
</MODELS>
```

Parameter XML File

Quantum Lattice Model

application programs: **Quantum Monte Carlo** | **Exact Diagonalization** | **DMRG** | **DMFT**

Outputs in HDF5 & XML

Python based evaluation tools

Plots

Infrastructure for International Collaboration

World-wide Workshops
- Developers Workshop
- Users Workshop, Summar School

Mailing Lists
- ALPS developers mailing list
- ALPS users mailing list

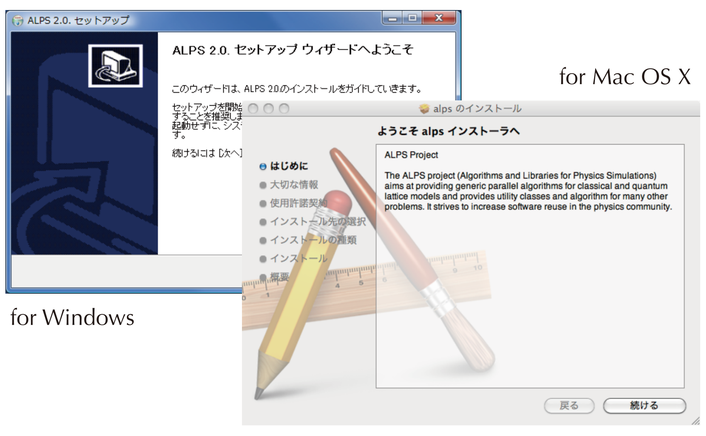
Source Code Management System
- SVN (Subversion)

Bug Tracking System
- Trac

Web Page (Wiki)
- http://alps.comp-phys.org

Windows & Mac OS X Support

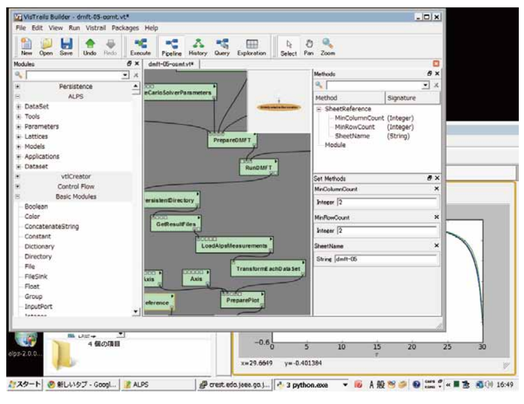
Ready-made Binary Installers



for Windows

ALPS + VisTrails

Integration with Workflow and Provenance Management System



http://www.vistrails.org/

Lisence Issue

The "cite-me" Lisence

Applications code
- published under ALPS Application Lisence
- free for non-commercial use
- based on GNU public license
- citation requirements

Library code
- less restrictive
- partially available under a free license

Modification/improvements of codes
- should be integrated into ALPS
- not obligatory to publish

ALPS Paper
- "The ALPS project release 2.0: open source software for strongly correlated systems", B. Bauer et. al., JSTAT P05001 (2011).

powered by ALPS
http://alps.comp-phys.org

contact:
Synge Todo <wistaria@phys.s.u-tokyo.ac.jp>
Department of Physics, University of Tokyo