The ALPS Project

Open Source Software for Strongly Correlated Systems

Matthias Troyer, ETH Zürich

for the ALPS collaboration

Overview and Introduction
Data formats
Future plans

The ALPS collaboration

ETH Zürich, Switzerland
- Philippe Corboz
- Emanuel Gull
- Munehisa Matsumoto
- Lode Pollet
- Matthias Troyer

IRRMA Lausanne, Switzerland
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RWTH Aachen, Germany
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- Salvatore Manmana

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Universität Stuttgart, Germany
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- Fabien Alet

TU Graz, Austria
- Franz Michel

UC Santa Barbara, USA
- Adrian Feiguin
- Simon Trebst

Columbia University, USA
- Philipp Werner

Honk Kong University, China
- Siegfried Gürtler

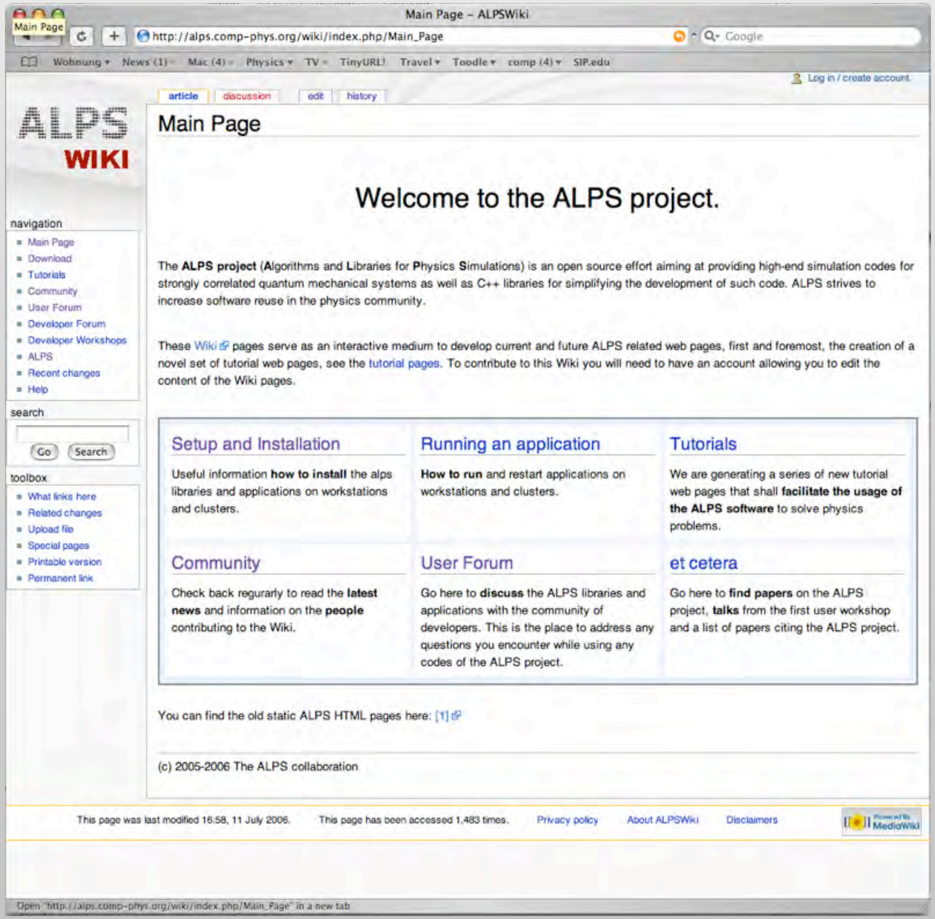
University of Tokyo, Japan
- Ryo Igarashi
- Synge Todo

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**



Simulation codes of quantum lattice models

- **The status quo**
  - individual codes
  - model-specific implementations
  - growing complexity of methods
- **ALPS**
  - community codes
  - generic implementations
  - simplified code development
  - common file formats

Key Technologies

Generic Programming in C++
- flexibility
- high-performance

Standard C++ Libraries
- fast development

XML / XSLT for Input/Output
- portability
- self-explanatory

MPI/OpenMP for Parallelization

Three 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. **Applications**
   - to be used also by non-experts
   - implement modern algorithms for a large class of models

The ALPS project

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

- The **simulation codes** include
  - Classical and Quantum Monte Carlo (path integrals, SSE)
  - Exact and Full Diagonalization
  - Density Matrix Renormalization Group (DMRG)
- **Motivation**
  - established algorithms
  - increased demand for reliable simulations from theorists and experimentalists

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

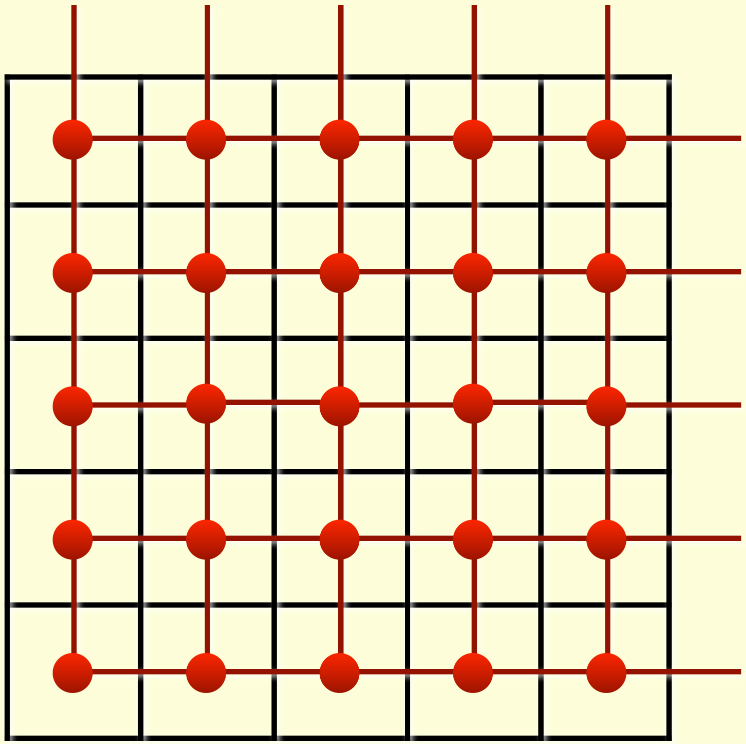
Quantum Monte Carlo | **Exact diagonalization** | **DMRG**

Results

The ALPS lattice library

A lattice

```
<LATTICEGRAPH name = "square lattice">
  <FINITELATTICE>
    <LATTICE dimension="2"/>
    <EXTENT dimension="1" size="L"/>
    <EXTENT dimension="2" size="L"/>
    <BOUNDARY type="periodic"/>
  </FINITELATTICE>
  <UNITCELL>
    <VERTEX/>
    <EDGE type="1">
      <SOURCE vertex="1" offset="0 0"/>
      <TARGET vertex="1" offset="0 1"/>
    </EDGE>
    <EDGE type="2">
      <SOURCE vertex="1" offset="0 0"/>
      <TARGET vertex="1" offset="1 0"/>
    </EDGE>
  </UNITCELL>
</LATTICEGRAPH>
```



The ALPS model library

A model

$$H_{XXZ} = \frac{J_{xz}}{2} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+) + J_z \sum_{\langle i,j \rangle} S_i^z S_j^z - h \sum_i S_1^z$$

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

<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"/>

<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>
```

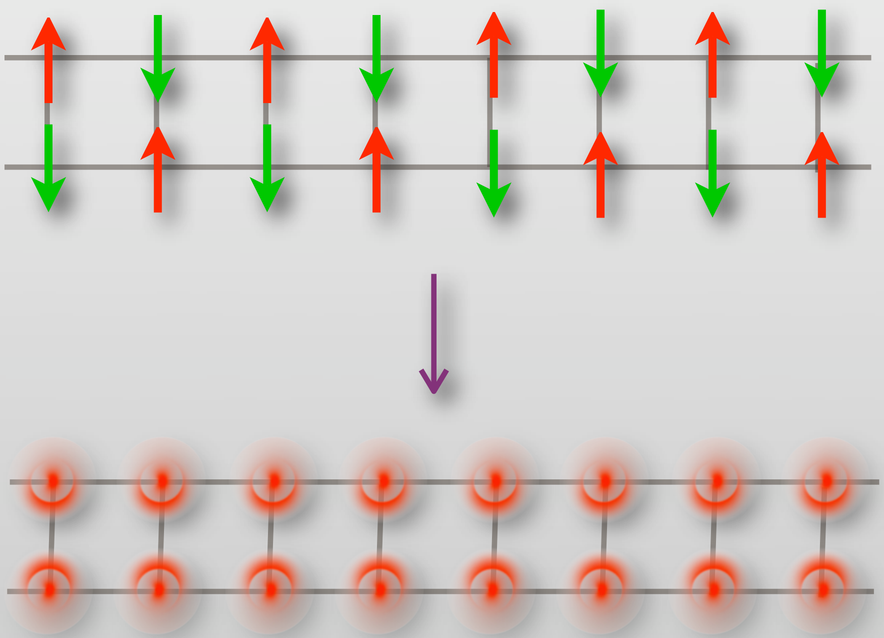
Current applications

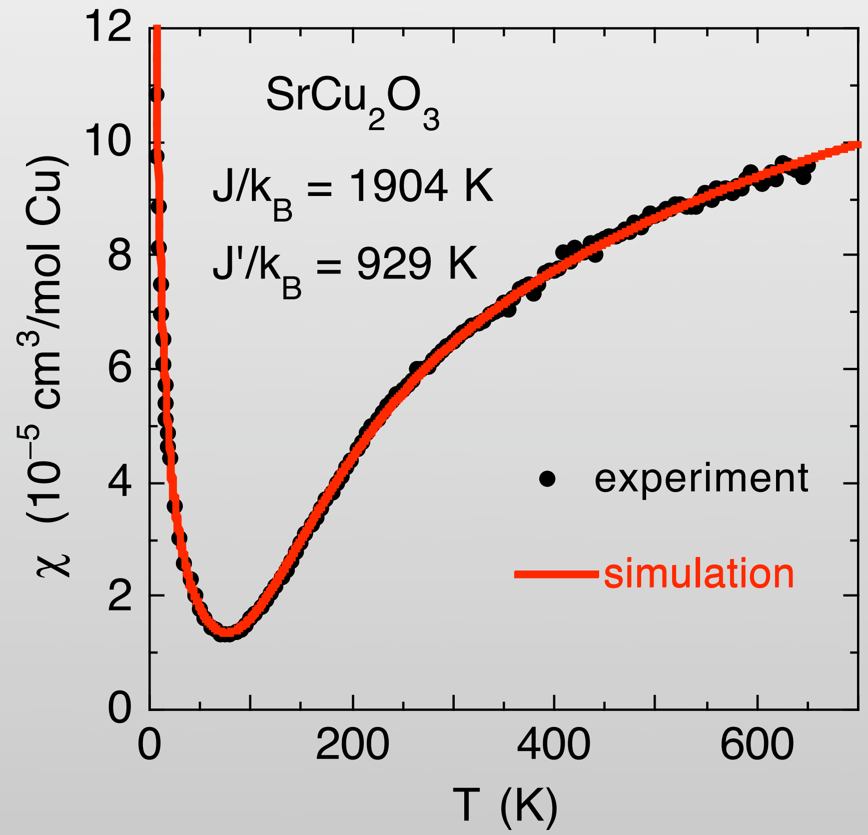
- **Classical Monte Carlo**
  - local and cluster updates for classical spin systems, M. Troyer
- **Quantum Monte Carlo**
  - stochastic series expansions (SSE), F. Alet, L. Pollet, M. Troyer
  - loop code for spin systems, S. Todo
  - continuous time worm code, S. Trebst, M. Troyer
  - extended ensemble simulations, S. Wessel, N. Stoop
- **Exact diagonalization**
  - full and sparse, A. Honecker, A. Läuchli, M. Troyer
- **DMRG**
  - single particle, S. Manmana, R. Noack, U. Schollwöck
  - interacting particles, A. Feiguin

Some applications of ALPS codes

- **Experimental data fitting**
  - Low-dimensional quantum magnets
  - Single molecule magnets
  - Ultracold bosonic atoms in optical traps
- **Theoretical predictions**
  - How to cool fermionic atoms in optical lattices well below T_F ?

Quantum spin ladders



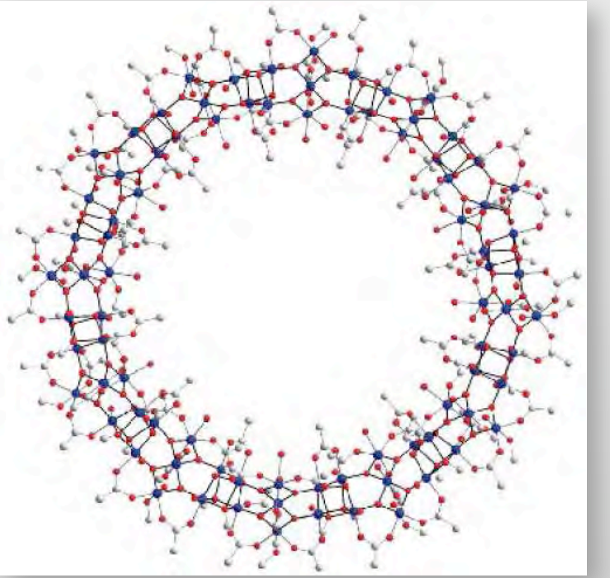


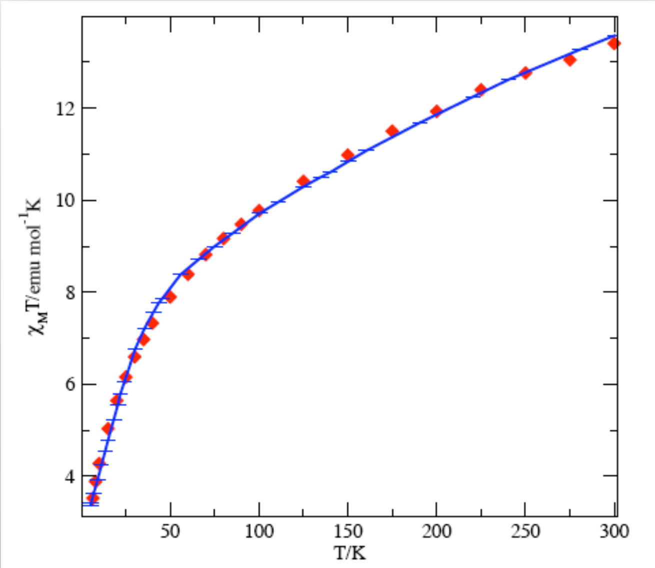
➡ compare microscopic models to experiments

Mn-84 molecules

Vassilis Tangoulis, in preparation

- How can we microscopically model interactions in Mn-84?





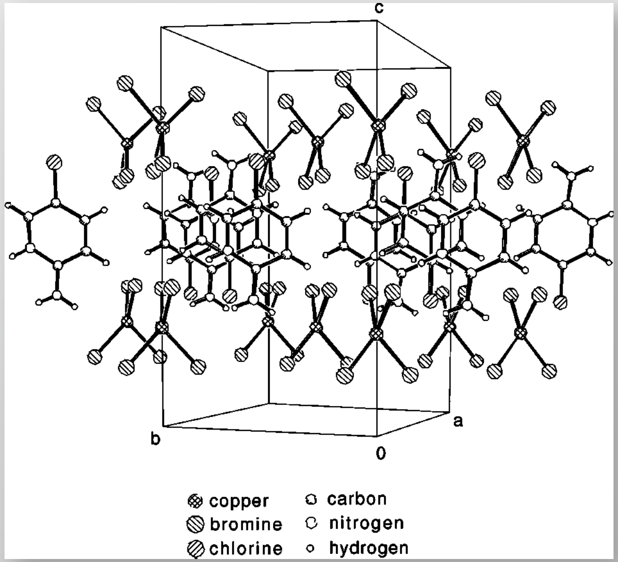
ALPS QMC codes

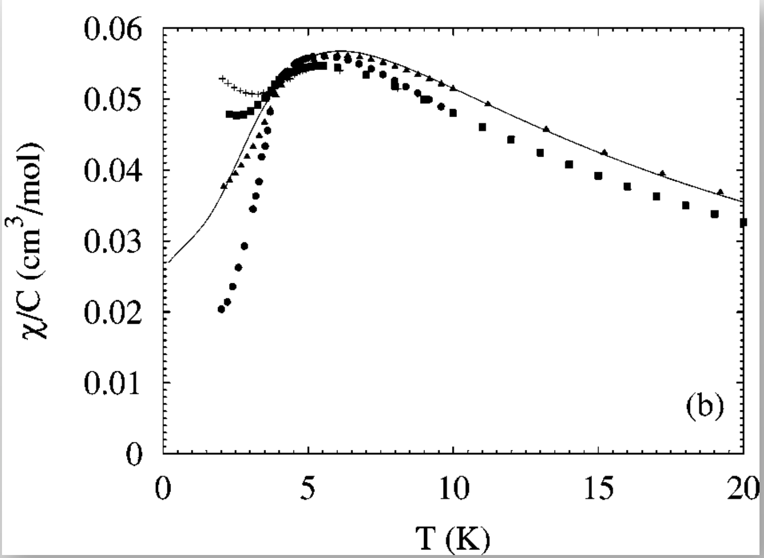
Numerical evaluation of susceptibility for full molecule:
Fit of magnetic interaction strength.

Low-dimensional quantum magnets

C.P. Landee et al., Phys. Rev. B **65**, 144412 (2002)

- How to characterize newly synthesized materials?

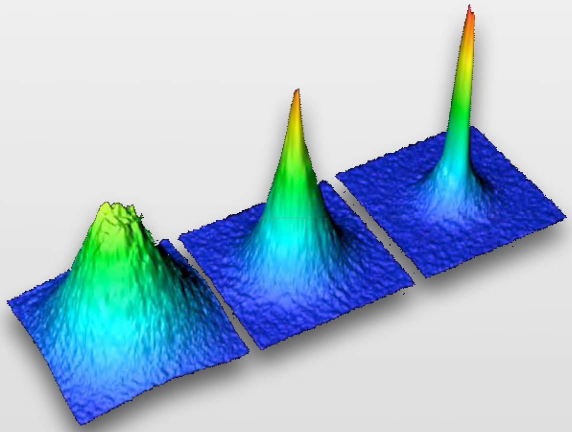




ALPS QMC codes

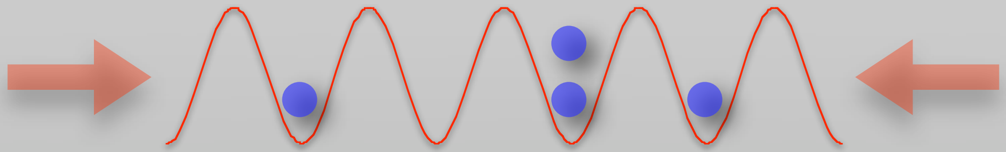
Numerical evaluation of susceptibility for 2D QHAF:
Fit of magnetic interaction strength.

BEC in ultracold atomic gases



T. Esslinger, ETH Zürich

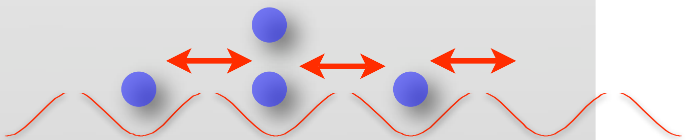
- Ultracold ^{87}Rb atoms form a Bose-Einstein condensate (BEC).
  - first observed in 1995
  - sympathetic cooling of fermionic ^{40}K atoms (2004)
- Standing laser waves form an optical lattice.



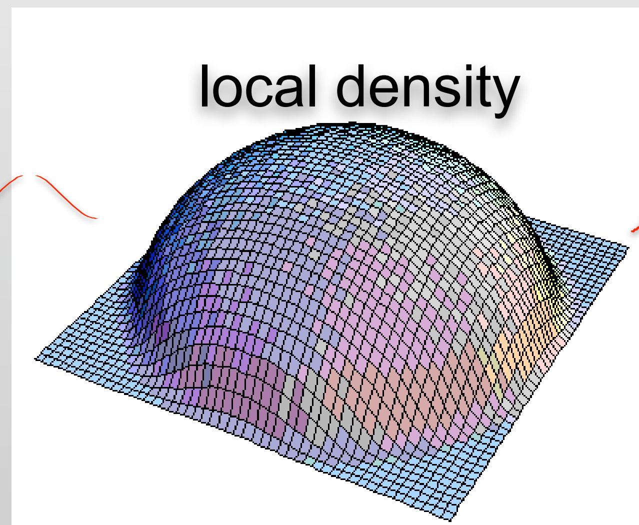
Realization of the Bose-Hubbard model

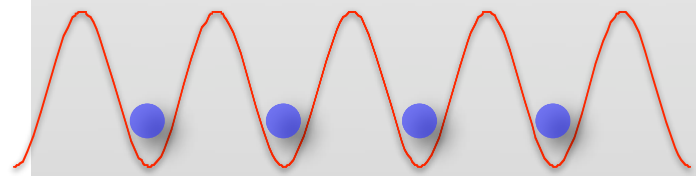
S. Wessel et al., Phys. Rev. A **70**, 053615 (2004)
O. Gygi et al., Phys. Rev. A **73**, 063606 (2006)

$$H = -t \sum_{\langle ij \rangle} \left(b_i^\dagger b_j + \text{h.c.} \right) + U \sum_i n_i (n_i - 1)/2 - \mu \sum_i n_i + V \sum_i r_i^2 n_i$$



suprafluid
coherent BEC





Mott-isolator
incoherent

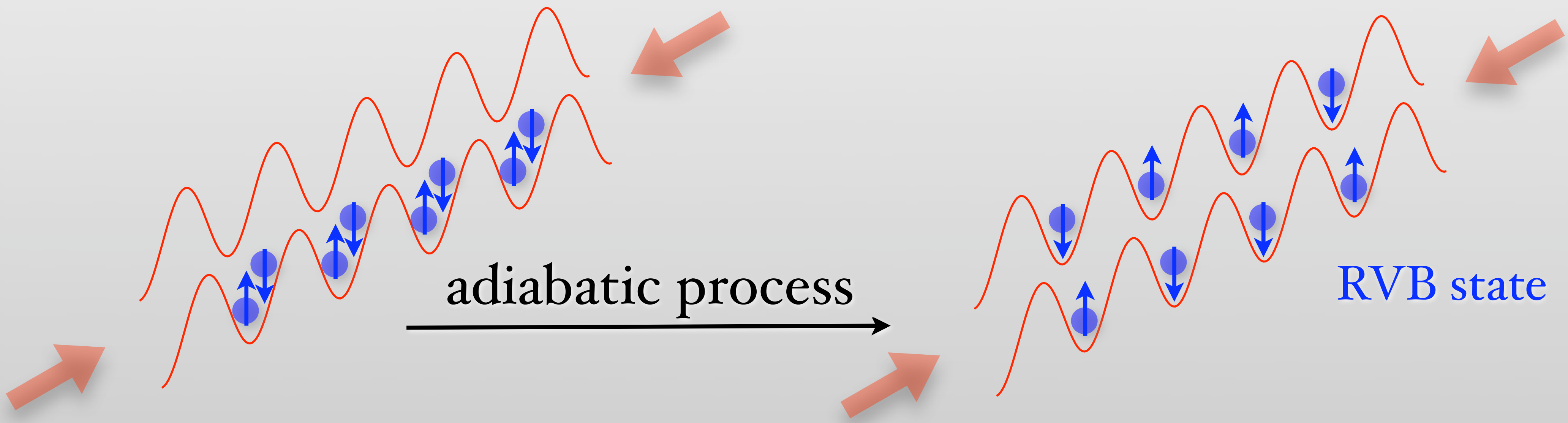
ALPS QMC codes

Numerical simulation of experimental setup:
60² sites and harmonic trapping potential

Ultracold fermionic atoms

S. Trebst *et al.*, Phys. Rev. Lett. **96**, 250402 (2006)

- How can we cool down fermions to some 0.01 T_F ?



ALPS exact diagonalization codes

Excitation spectra of intermediate states.

Time-evolution of proposed adiabatic processes.

Data Formats

XML

HDF-5

Three tiers of ALPS

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Common data formats

- are the most important part of the ALPS project
- Standard formats allow
  - uniform interface to all codes
  - exchange of simulation results
  - fighting data rot (files can still be understood after many years)
  - sharing analysis tools
  - archiving of raw data

Evaluating Monte Carlo data

- Reliable Monte carlo simulations need careful data analysis
  - equilibration effects
  - autocorrelation effects (binning analysis)
  - crosscorrelation effects (jackknife or bootstrap method)
- Common formats encourage development and sharing of good and flexible analysis tools

Archiving Monte Carlo data

- We want the raw Monte Carlo data (time series) to be available and accessible even after the PhD student finishes his thesis and leaves
- Standard data formats will simplify
  - Archiving of results with data rot in archive server
  - Easy searching and retrieval
  - Publication of results with papers, as auxiliary electronic material

Validating applications

- Careful and systematic validation simulation programs is an often overlooked problem (Laughlin, Kadanoff)
- Set up a suite of benchmark problems with verified results
  - use it manually in debugging phase of your own program
  - use it automated to run regular validation and regression testing when
    - porting to new compilers
    - porting to new machines
    - changing library or operating system versions

Monte Carlo data format standards workshop

- Zürich, September 11, 2006
- Agenda
  - collect experiences
  - define standard formats
  - discuss evaluation and archiving
- Confirmed participants:
  - F.F. Assaad, A. Läuchli, B. Bernu, D. Ceperley, J.N. Kim, D.P. Landau, T. Schulthess, M. Troyer, S. Wessel, ...
- Your participation is welcome: http://xml.comp-phys.org

New Features

Integration with band structure codes
Dynamical Mean Field Theory framework
Release plans

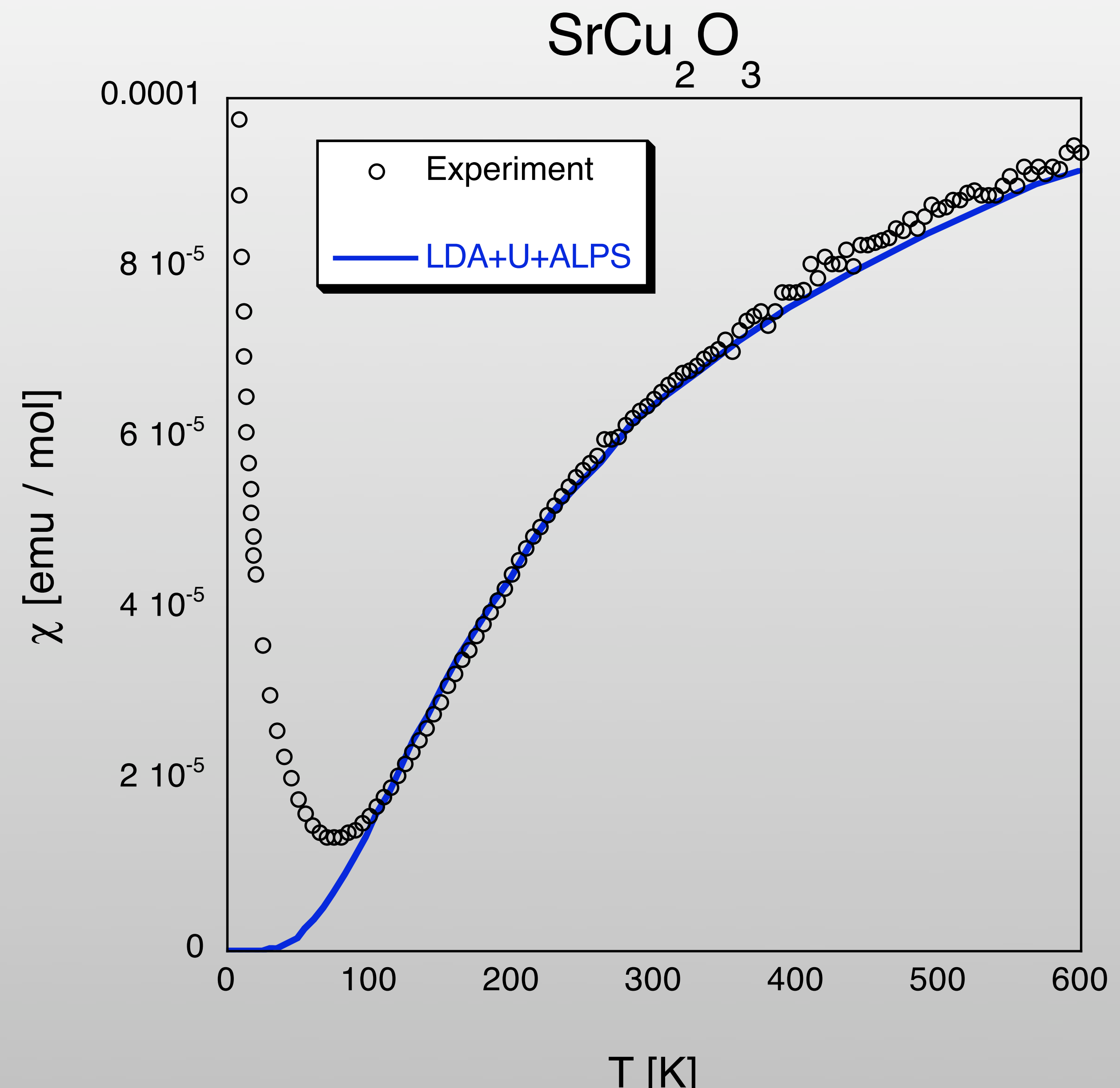
Ab-initio simulations of quantum magnets

- Simulate realistic magnetic models instead of toy models
  - obtain microscopic exchange constants from LDA+U
  - simulate quantum spin models using these exchange constants
- Was done by hand in the past
  - CaV_2O_3, MgV_2O_3, CaV_3O_7, CaV_4O_9
  - Korotin, Elfimov, Anisimov, Troyer and Khomskii, PRL '99
- Can we automate this?

ALPS Interface to band structure codes

- ORNL is developing standard XML I/O data formats and helper libraries for band structure codes
- Implementation in Stuttgart TB-LMTO-ASA band structure code by Anton Kozhevnikov (Ekaterinburg)
- Simple helper tool by Anton Kozhevniko creates ALPS input file (lattice structure, model Hamiltonian) from XML output of LDA+U code
- Automated workflow from crystal structure to magnetic properties

Example: $SrCu_2O_3$

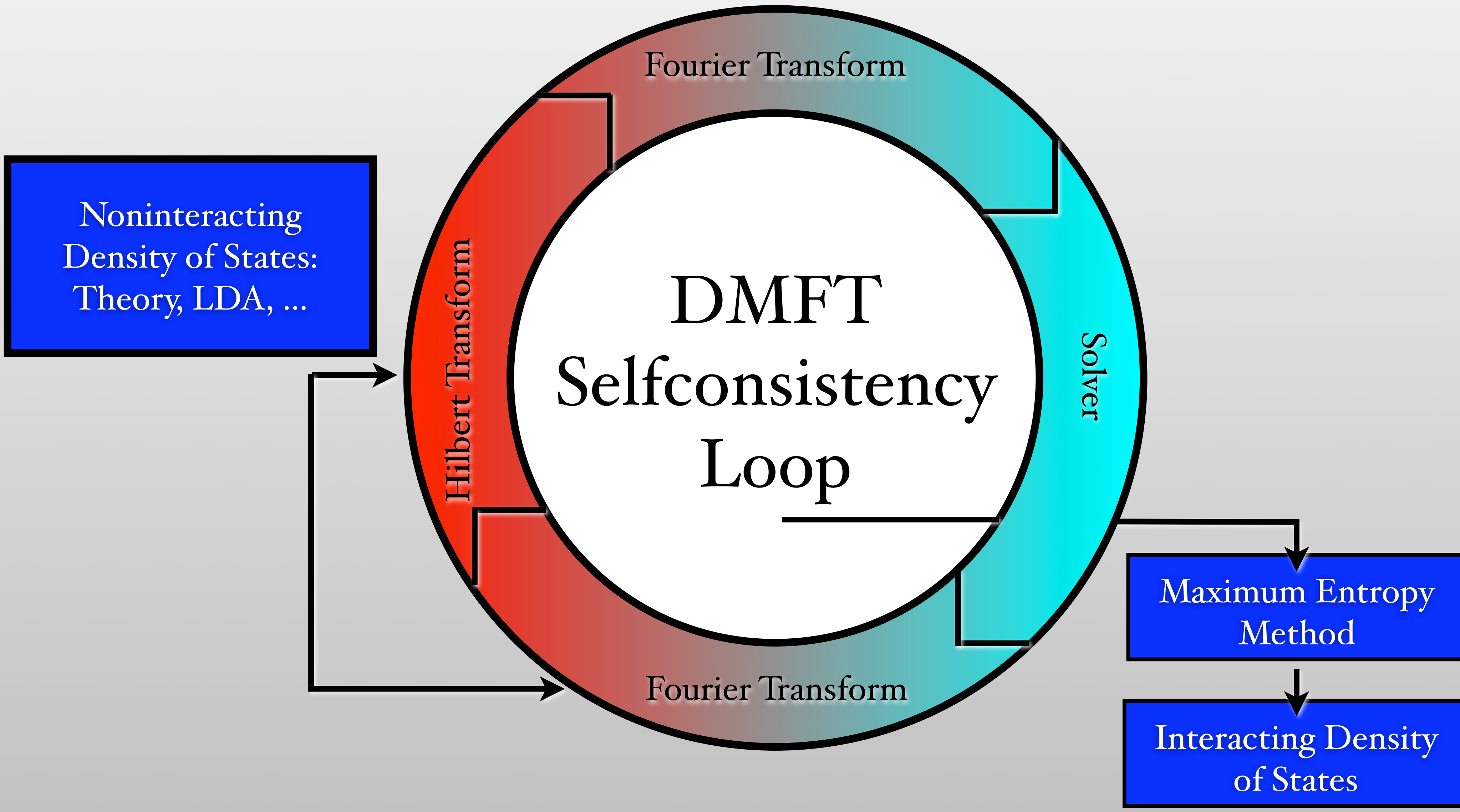


Dynamical Mean Field Theory

- E. Müller-Hartmann, Z. Phys. B **74** 507 (1989).
  M. Metzner and D. Vollhard, PRL **62**, 324 (1989).
  A. Georges and G. Kotliar Phys. Rev. B **45**, 6479 (1992).
  A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).
  T. Maier *et al.*, Rev. Mod. Phys. **77**, 1027 (2005).

- is an approximative but successful method for describing strongly interacting fermions in high dimensions
- solves a few - site problem in the presence of a self-consistent bath provided by the rest of the system

DMFT self-consistency loop



ALPS DMFT framework

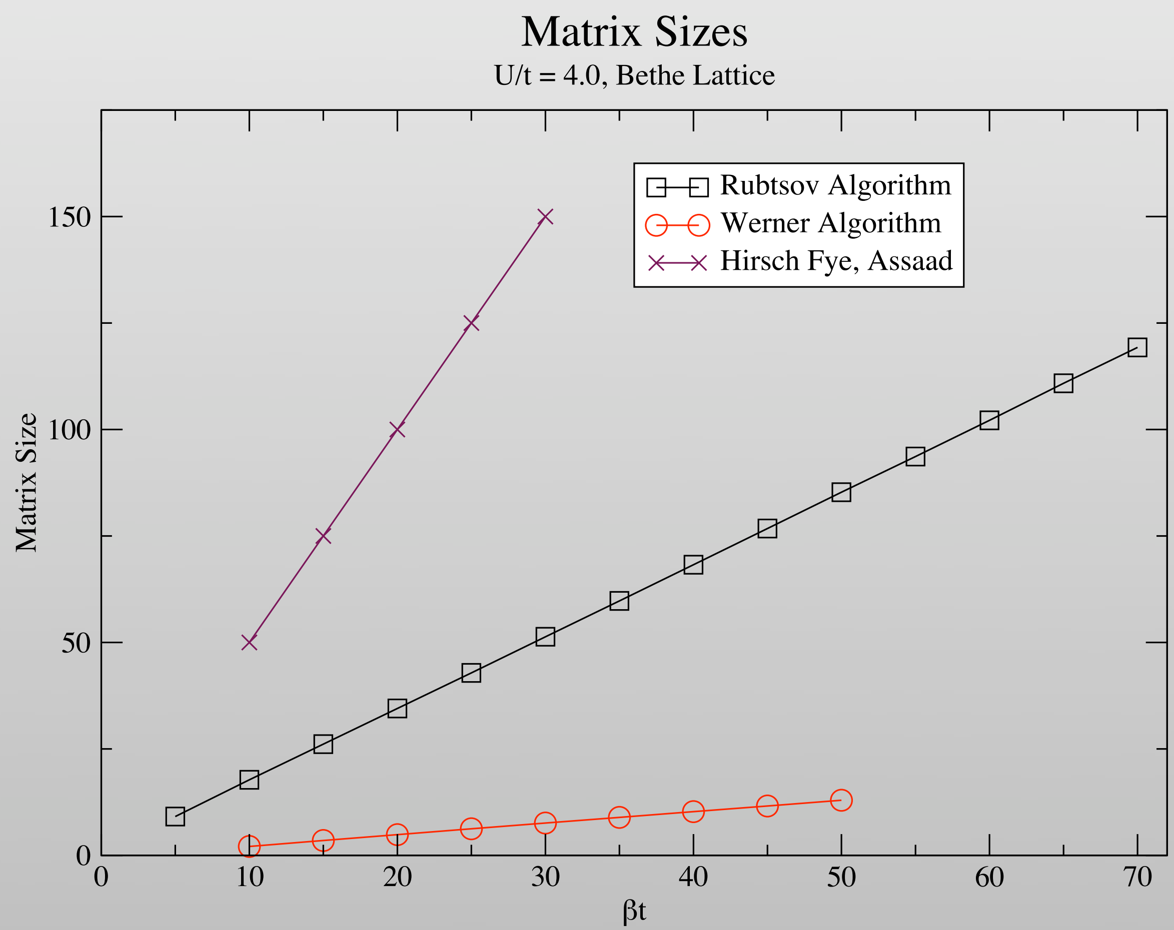
- Provides a modular system for solving the DMFT equations
  - Fourier transforms
  - Hilbert transforms
  - Impurity solvers
- plug-in based:
  - can use ALPS components
  - or user - provided external components written in any language
- work in progress on establishing standard data formats
  - workshop November 2006 in Göttingen, Germany

ALPS DMFT QMC solvers

- So far we have implemented three QMC solvers
  - Hirsch-Fye algorithm (Hirsch, J. E., and R. M. Fye, PRL '86)
  - Rubtsov *et al.* continuous time expansion in U (PRB '05)
  - Werner *et al.* continuous time expansion in t (PRL, in press)
- Performed accuracy tests and performance comparisons
  - Gull *et al*, in preparation
  - see talk by Philipp Werner at the workshop

Solver Comparison

- close to Mott transition: Werner *et al.* solver is
  - 10^6 times faster than Hirsch-Fye
  - 10^3 times faster then Rubtsov *et al.* solver



Release plans

- Release 1.3, fall 2006
  - Translation symmetry in diagonalizaton codes
  - Custom measurements of static quantities
  - new application: DMRG
- Release 1.4, summer 2007
  - multi-site terms in Hamiltonian and measurements
  - measurement of dynamic quantities
  - GUI for lattice construction
  - support for Cray XT3 and IBM BlueGene/L

Plans for ALPS 2.0

- New applications
  - Full integration of DMFT
  - Continuum QMC
- New features
  - Full support for point group symmetries
  - Interface with band structure codes
  - Application validation benchmarks
  - Archiving server
  - Support for Windows
  - Scripting using Python

Conclusions

- Open source codes for strongly correlated systems intended for non-experts: what do you need?
- Setting standard for data formats to enable
  - common input formats
  - sharing of results
  - sharing of evaluation tools
  - archiving of results
  - validating simulation programs
  - workshop: Sept. 11, 2006 in Zürich

http://alps.comp-phys.org

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