HFM-ESF Trieste '07

Introduction to ALPS

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

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for the ALPS Collaboration

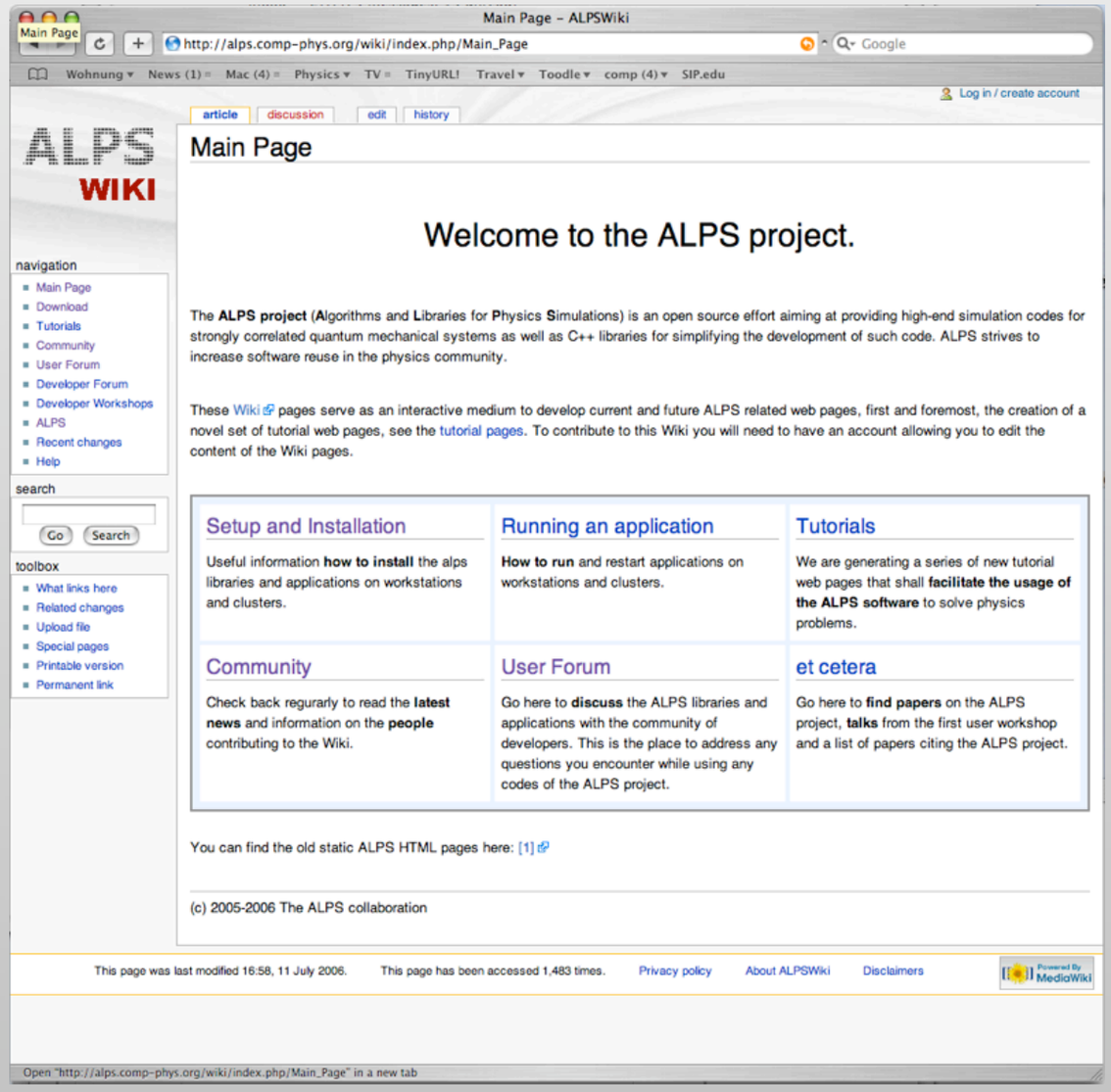
based on talks by M. Troyer & S. Todo

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**



The ALPS collaboration

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- Emanuel Gull
- Munehisa Matsumoto
- Lode Pollet
- Matthias Troyer

IRRMA / EPF Lausanne, Switzerland
- Andreas Läuchli
- Salvatore Manmana

RWTH Aachen, Germany
- Ulrich Schollwöck
- Ian McCulloch

Universität Marburg, Germany
- Reinhard Noack

Universität Göttingen, Germany
- Andreas Honecker
- Thomas Pruschke

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TU Graz, Austria
- Franz Michel

UC Santa Barbara, USA
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- Simon Trebst

Columbia University, USA
- Philipp Werner

Honk Kong University, China
- Siegfried Gürtler

University of Tokyo, Japan
- Ryo Igarashi
- Synge Todo

Outline

- Overview of the ALPS project
- ALPS libraries and applications
- ALPS and XML
- Tutorial(s)

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- International collaboration for developing open-source softwares for simulation of quantum lattice models, such as quantum spin systems, electron systems, etc
- ALPS Libraries = collection of generic C++ libraries
- ALPS Applications = collection of application packages using modern algorithms such as QMC, DMRG, ED, etc

The status quo

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- No “community codes” available
  - Individual code for each project
  - Model specific implementations

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  - Model specific implementations
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  - Weeks to months of software development
- Inputs/Outputs in non-portable formats

Target audience

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- Experimental physicists
  - Use “canned codes” to model materials
  - Determine microscopic parameters by fitting experimental data to simulations

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- Experimental physicists
  - Use “canned codes” to model materials
  - Determine microscopic parameters by fitting experimental data to simulations
- Theoretical physicists
  - Quick check of theoretical ideas using many modern algorithms
    - Monte Carlo, Diagonalization, DMRG, ...
    - Also useful for debugging
  - Libraries simplify and accelerate code development

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

ALPS - Platforms

- Unix Flavors:
  Linux (Fedora,...) , AIX, HP-UX, IRIX, ...
- Windows:
  Cygwin, CoLinux
- MacOS X
- High performance machines:
  Cray XT-3, IBM BlueGene/L

The "cite me" license

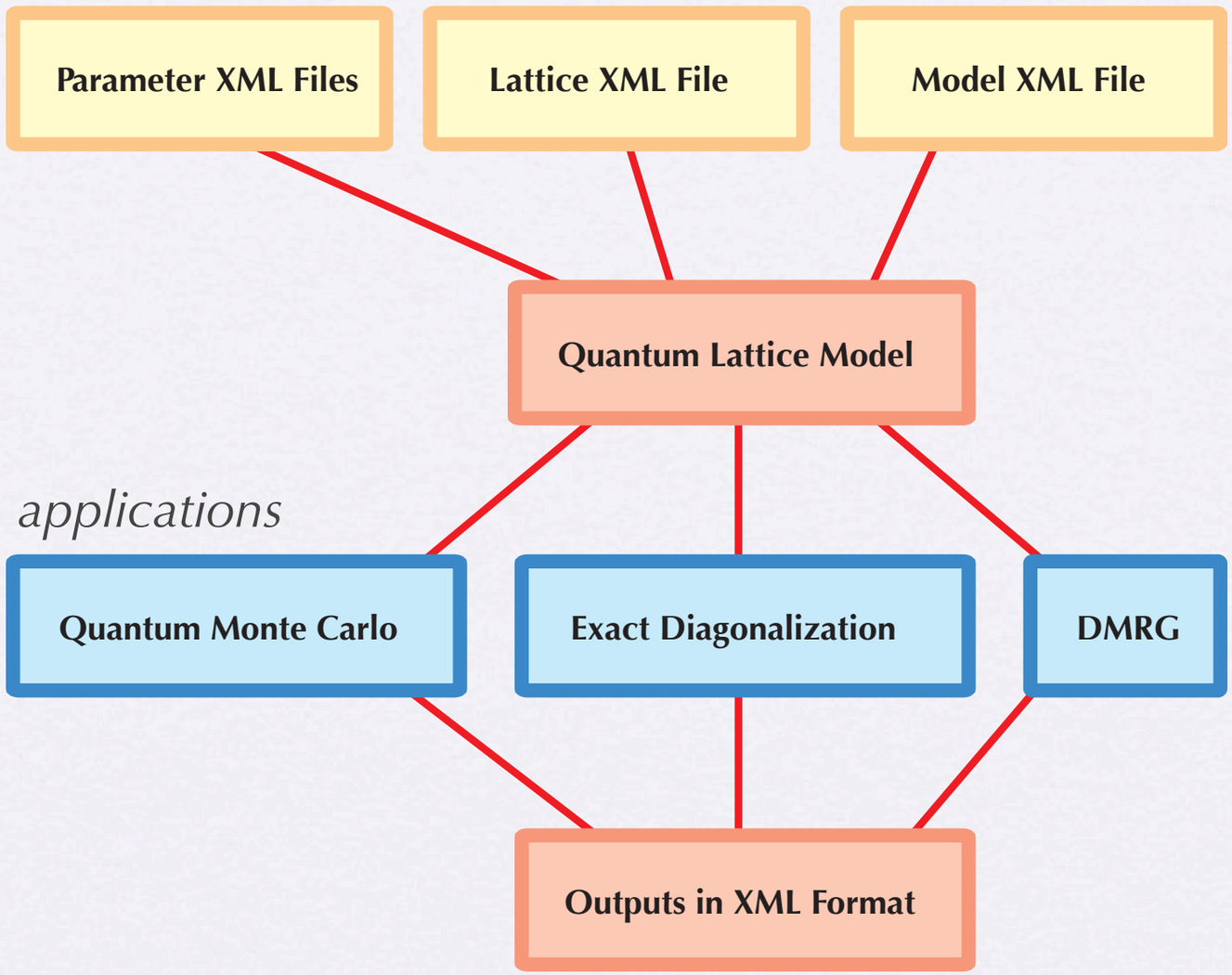
- "ALPS Application License" for applications
  - free for non-commercial use
  - based on GNU public license
  - citation requirements
- "ALPS Library License" for library codes
  - less restrictive
  - partially available under a (BSD-like) free license as "ALPS Light Libraries"
- Read "LICENSE.txt" for more detail
- Most recent ALPS paper:

A.F. Albuquerque, et al, (for the ALPS collaboration),
The ALPS project release 1.3: open source software for strongly correlated systems,
J. Magn. Mag. Mat. **310**, 1187 (2007) (JMMM).

XML and ALPS

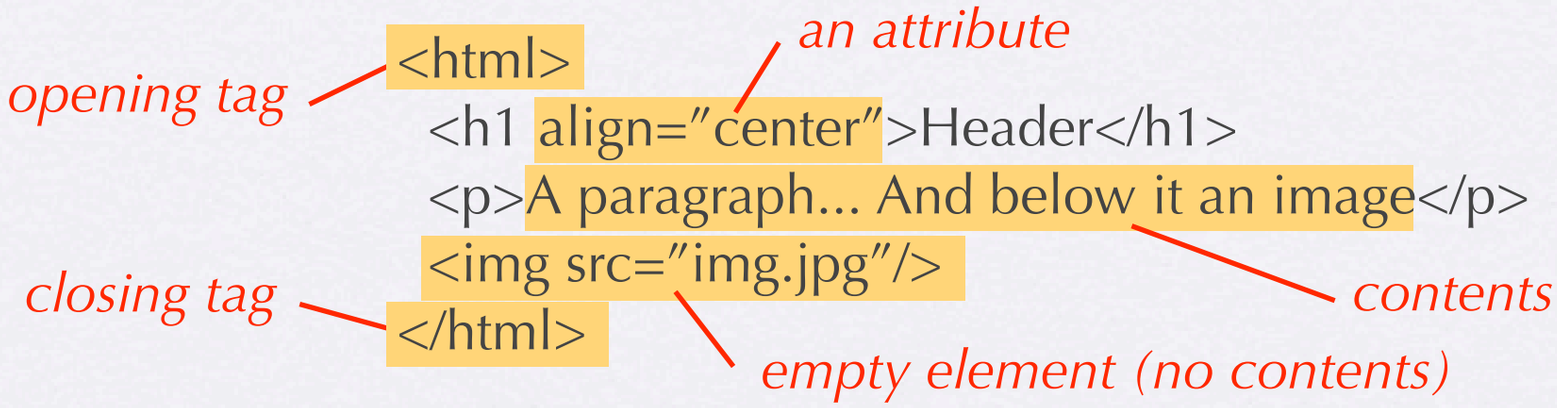
- XML basics
- Input/Output of simulations in XML format
- Lattice/Model XML
- Running simulations in ALPS

Simulations with ALPS



XML basics

- XML = eXtensible Markup Language
- A flexible way to create well-formed and self-describing data
- We use "tags" to describe the structure of documents
  - Example: HTML (XHTML)



ALPS tool: parameter2xml

parameter sets in a compact form

```
LATTICE_LIBRARY=”lattices.xml”;
LATTICE=”chain lattidce”;
MODEL_LIBRARY=”models.xml”;
MODEL="spin";
THERMALIZATION=10000;
SWEEPS=1000000;
L=128;
{ T=0.2; }
{ T=0.4; }
{ T=0.6; }
{ T=0.8; }
{ T=1.0; }
```

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task-specific parameters

parameter2xml

myjob.in.xml

myjob.task1.in.xml

myjob.task2.in.xml

myjob.task3.in.xml

myjob.task4.in.xml

myjob.task5.in.xml

Lattice XML (1/3)

definition of basis vectors

```
<LATTICES>
  <LATTICE name="square lattice" dimension="2">
   <PARAMETER name="a" default="1"/>
   <BASIS>
     <VECTOR>a 0</VECTOR>
     <VECTOR>0 a</VECTOR>
   </BASIS>
   <RECIPROCALBASIS>
     <VECTOR>2*pi/a 0</VECTOR>
     <VECTOR>0 2*pi/a</VECTOR>
   </RECIPROCALBASIS>
  </LATTICE>
  ...
```

Lattice XML (2/3)

definition of the unit cell

```
<LATTICES>
 <LATTICE name="square lattice" dimension="2">
   ...
 </LATTICE>
 <UNITCELL name="simple2d" dimension="2">
   <VERTEX/>
   <EDGE>
     <SOURCE vertex="1" offset="0 0"/>
     <TARGET vertex="1" offset="0 1"/>
   </EDGE>
   <EDGE>
     <SOURCE vertex="1" offset="0 0"/>
     <TARGET vertex="1" offset="1 0"/>
    </EDGE>
</UNITCELL>
...
```

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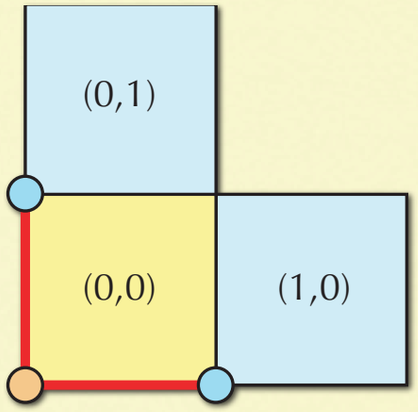
     <TARGET vertex="1" offset="0 1"/>
   </EDGE>
   <EDGE>
     <SOURCE vertex="1" offset="0 0"/>
     <TARGET vertex="1" offset="1 0"/>
    </EDGE>
 </UNITCELL>
 ...
```



Lattice XML (3/3)

specifying lattice size and boundary conditions

```
<LATTICES>
  <LATTICE name="square lattice" dimension="2">
    ...
  </LATTICE>
  <UNITCELL name="simple2d" dimension="2">
    ...
  </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 (1/2)

definition of local basis and operators

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

Model XML (2/2)

definition of model Hamiltonian

```
<MODELS>
  <BASIS name="spin">
    ...
  </BASIS>
  <OPERATOR name="Sz" matrixelement="Sz"/> ...
  <HAMILTONIAN name="spin">
    <PARAMETER name="Jz" default="1"/>
    <PARAMETER name="Jxy" default="1"/>
    <PARAMETER name="h" default="0"/>
    <BASIS ref="spin"/>
    <SITETERM>-h*Sz</SITETERM>
    <BONDTERM source="i" target="j">
      Jz*Sz(i)*Sz(j) +
      Jxy/2*(Splus(i)*Sminus(j)+Sminus(i)*Splus(j))
    </BONDTERM>
  </HAMILTONIAN>
</MODEL>
```

Model XML (2/2)

definition of model Hamiltonian

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

```
<MODELS>
  <BASIS name=
    ...
  </BASIS>
  <OPERATOR name="Sz" matrixelement="Sz"/> ...
  <HAMILTONIAN name="spin">
    <PARAMETER name="Jz" default="1"/>
    <PARAMETER name="Jxy" default="1"/>
    <PARAMETER name="h" default="0"/>
    <BASIS ref="spin"/>
    <SITETERM>-h*Sz</SITETERM>
    <BONDTERM source="i" target="j">
      Jz*Sz(i)*Sz(j) +
      Jxy/2*(Splus(i)*Sminus(j)+Sminus(i)*Splus(j))
    </BONDTERM>
  </HAMILTONIAN>
</MODEL>
```

- More examples for lattice and model XMLs can be found at

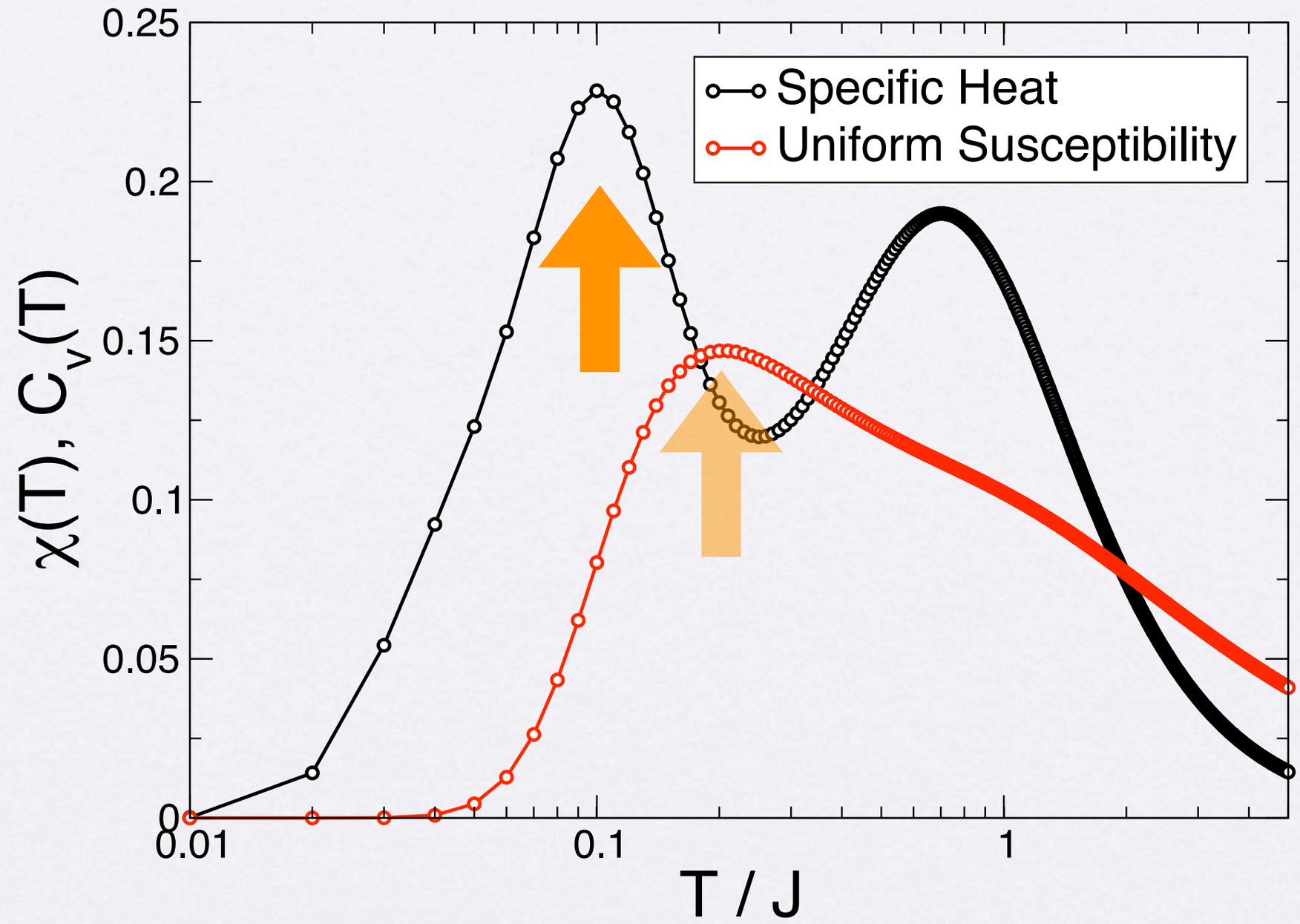
  $HOME/ALPS/lib/xml/lattices.xml

  chain, ladder,
  square, triangular, hexagonal,
  simple cubic, bcc, fcc, etc

  $HOME/ALPS/lib/xml/models.xml

  spin, hardcore boson,
  boson Hubbard, fermion Hubbard,
  Kondo lattice models, etc

Thermodynamics of a 12 sites S=1/2 Kagome system



Dive into the mysteries of the S=1/2 Kagome system ...

- Find the instructions for the tutorial here:
  http://irrmawww.epfl.ch/scs/HFM-Tutorial.html

- Further information on ALPS
  http://alps.comp-phys.org/

Enjoy!