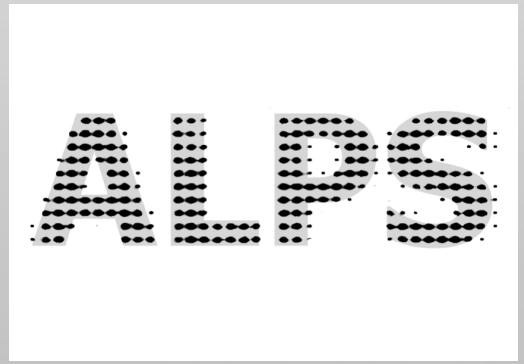
The ALPS Project

Open Source Software for Quantum Lattice Models

Simon Trebst, ETH Zürich

The ALPS collaboration



http://alps.comp-phys.org

The ALPS collaboration

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

ETH Zürich, Switzerland
- Fabien Alet
- Prakash Dayal
- Mathias Körner
- Guido Schmid
- Simon Trebst
- Matthias Troyer
- Philipp Werner
- Stefan Wessel

Universität Marburg, Germany
- Reinhard Noack
- Salvatore Manmana

Universität Würzburg, Germany
- Martin Jöstingmeier

University of Tokyo, Japan
- Synge Todo

Université de Toulouse, France
- Andreas Läuchli

RWTH Aachen, Germany
- Ulrich Schollwöck
- Ian McCulloch

Universität Bonn, Germany
- Axel Grzesik

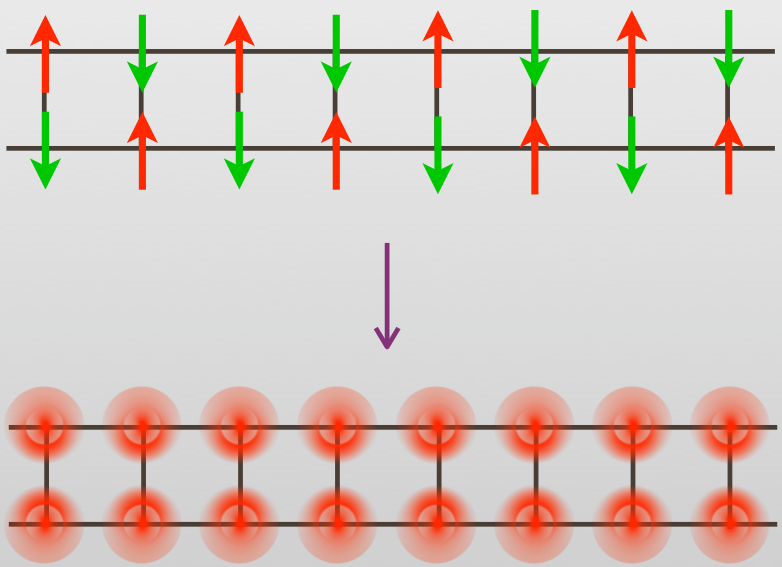
TU Graz, Austria
- Franz Michel
- Hans-Gerd Evertz

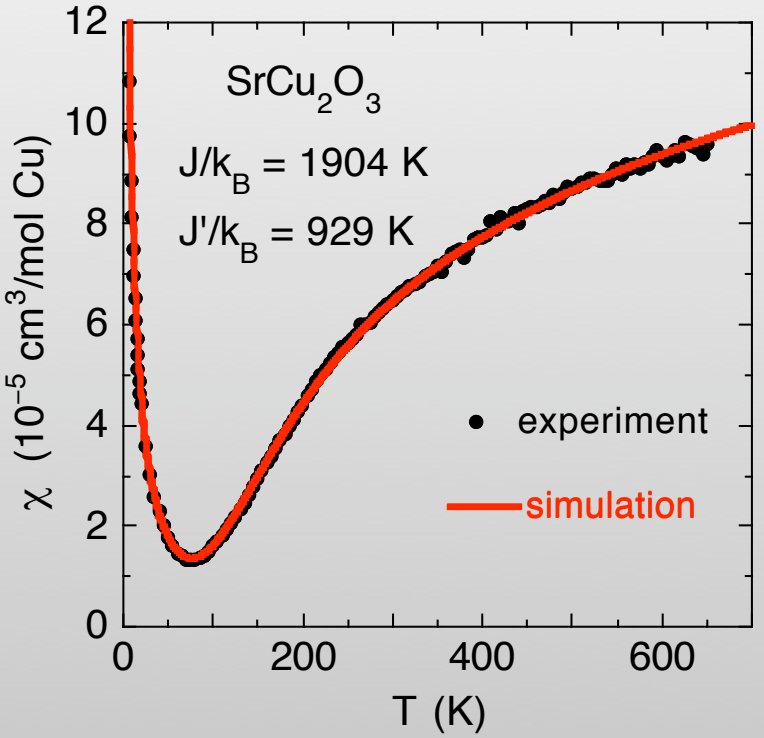
TU Braunschweig, Germany
- Andreas Honecker

The ALPS project

- open source libraries and simulation codes for strongly correlated quantum systems
  - Quantum Monte Carlo
  - exact diagonalization
  - DMRG
- Motivation
  - established algorithms
  - increased demand for reliable simulations from theorists and experimentalists

Strongly correlated systems



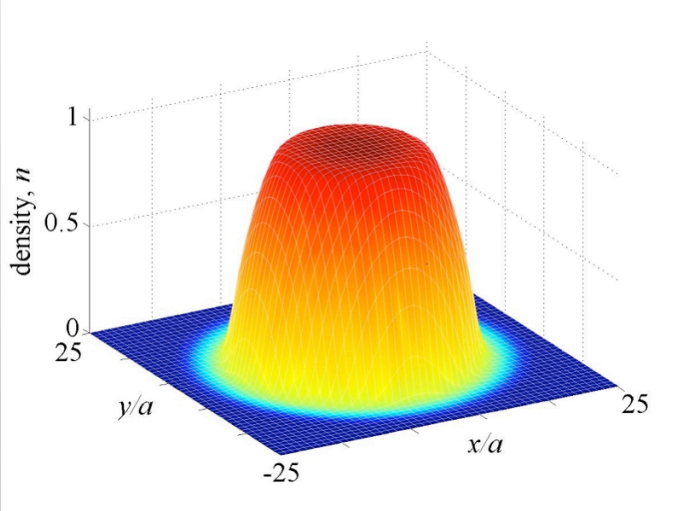


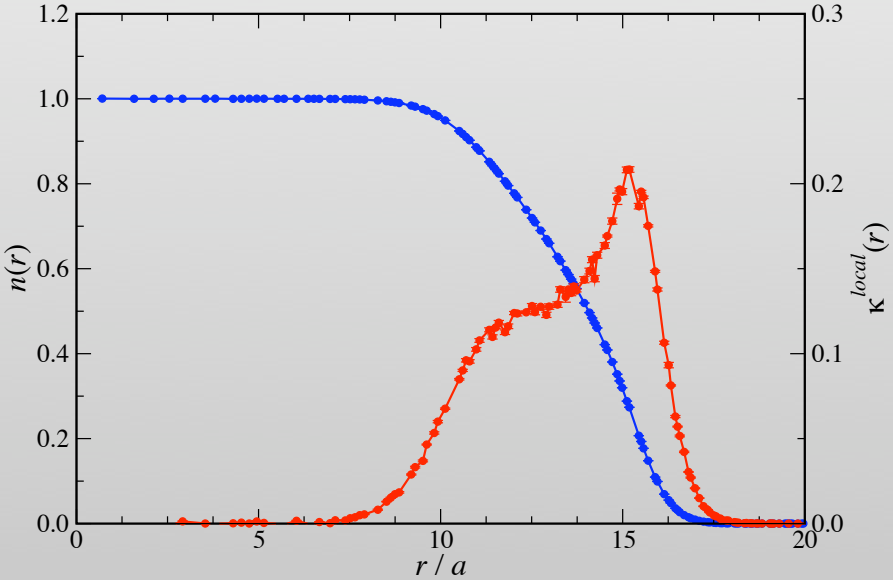
➡ compare microscopic models to experiments

Strongly correlated systems

talk H28.004 by Stefan Wessel

- BEC of ultra-cold atoms in optical lattices





➡ quickly test theoretical ideas

Simulation of quantum lattice models

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

Modern technologies

- **"Starting late" allows us to use**
  - generic programming in C++
    ➡ fast & flexible codes
  - standard C++ libraries
  - MPI and OpenMP for parallelization
  - XML / XSLT for file processing

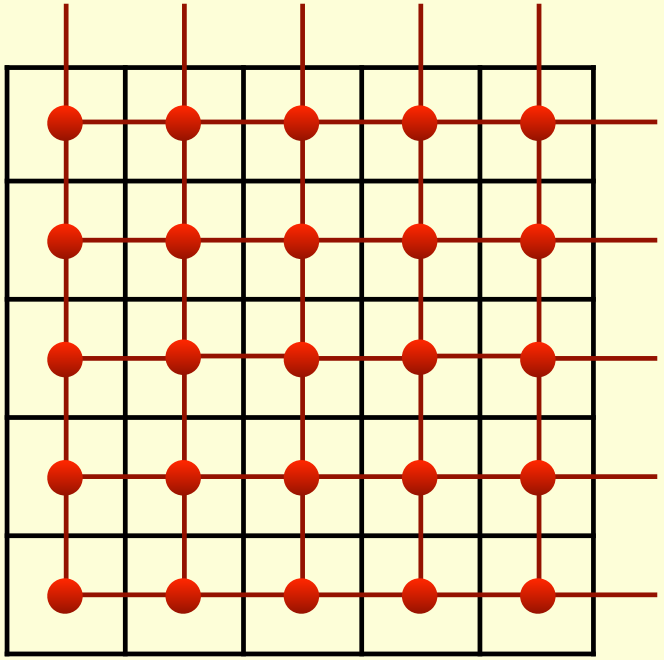
The ALPS sources

applications	QMC	ED	DMRG	...
domain specific libraries	lattice	model	observables	scheduler
numerics	random	ublas	IETL	
general C++	graph		serialization	XML/XSLT
C / Fortran	BLAS	LAPACK	MPI	

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>
```

Simulations with ALPS

Lattice

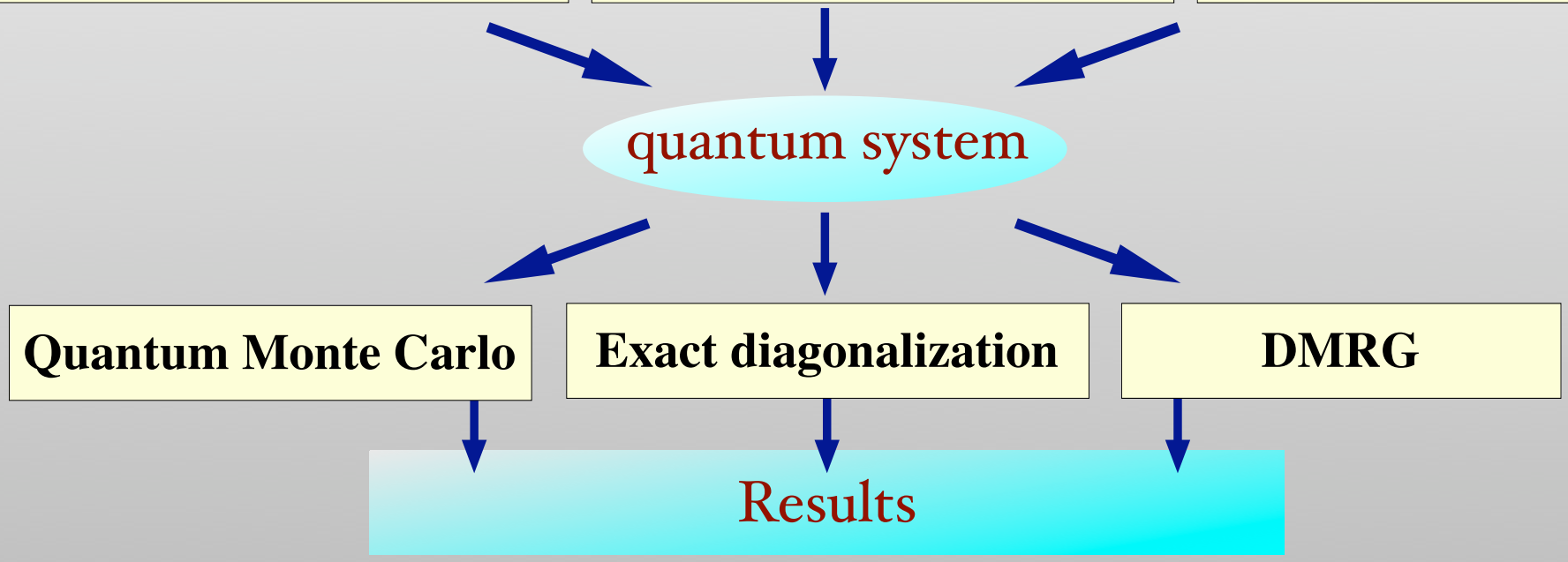
```
<LATTICEGRAPH name = "square lattice">
  <FINITELATTICE>
    <LATTICE dimension="2"/>
    <EXTENT dimension="1" size="L"/>
    <EXTENT dimension="2" size="L"/>
    <BOUNDARY type="periodic"/>
  </FINITELATTICE>
  <UNITCELL>
    ...
  </UNITCELL>
</LATTICEGRAPH>
```

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

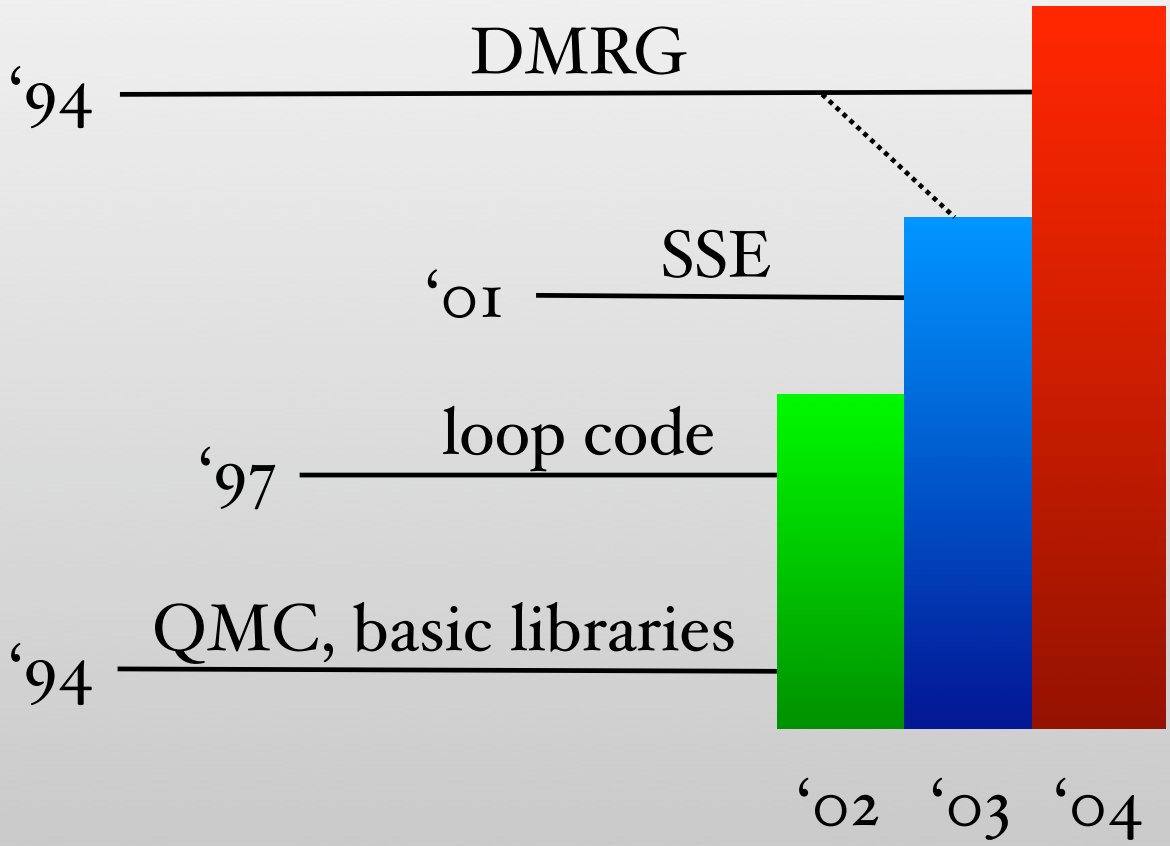
```
LATTICE = “square lattice”
L = 100

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

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



Open source development of ALPS

- Collaborative development
- Why open source codes?
- License discussion
- Funding situation

The History



the dark age

ALPS

Current applications

- **Quantum Monte Carlo**
  - stochastic series expansions (SSE), F. Alet, M. Troyer
  - loop code for spin systems, S. Todo
  - continuous time worm code, S. Trebst, M. Troyer
- **Exact diagonalization**
  - full and sparse, A. Honecker, A. Läuchli, M. Troyer
- **DMRG**
  - single particle, S. Manmana, R. Noack, U. Schollwöck
  - interacting particles, I. McCulloch

Collaborative development

Austria, France, Germany, Japan, Netherlands and Switzerland

- Some 15 developers, mostly PhDs.
- technical infrastructure
  - source code control system (CVS)
  - mailing lists
  - web page
- semi-annual workshops

Developer workshops

- Developers meet at semi-annual workshops
  - review of finished projects
  - discussion of current developments
  - road-map for new developments in the next 6 months
- Workshop are essential to coordinate and drive the development.

Open source codes

- **Why open source?**
  - community profits from improvements by individual developers

    e.g. adding disorder to models
  - simplify code development

    build on lattice, model, ... libraries
  - non-experts can use sophisticated algorithms
  - reproducibility of published scientific results

Open source codes

open sources ⟷ **scientific return**

- **Why should a researcher publish his codes?**
  - start new collaborations / networks
  - name recognition
  - citations
  - peer pressure to contribute
- **The “cite me” - license**

The “cite me” - license

- **Applications codes**
  - free for non-commercial applications
  - based on GNU public license
  - citation requirements
- *Modifications / improvements* of codes
  - should be integrated into ALPS
  - not obligatory to publish

The “cite me” - license

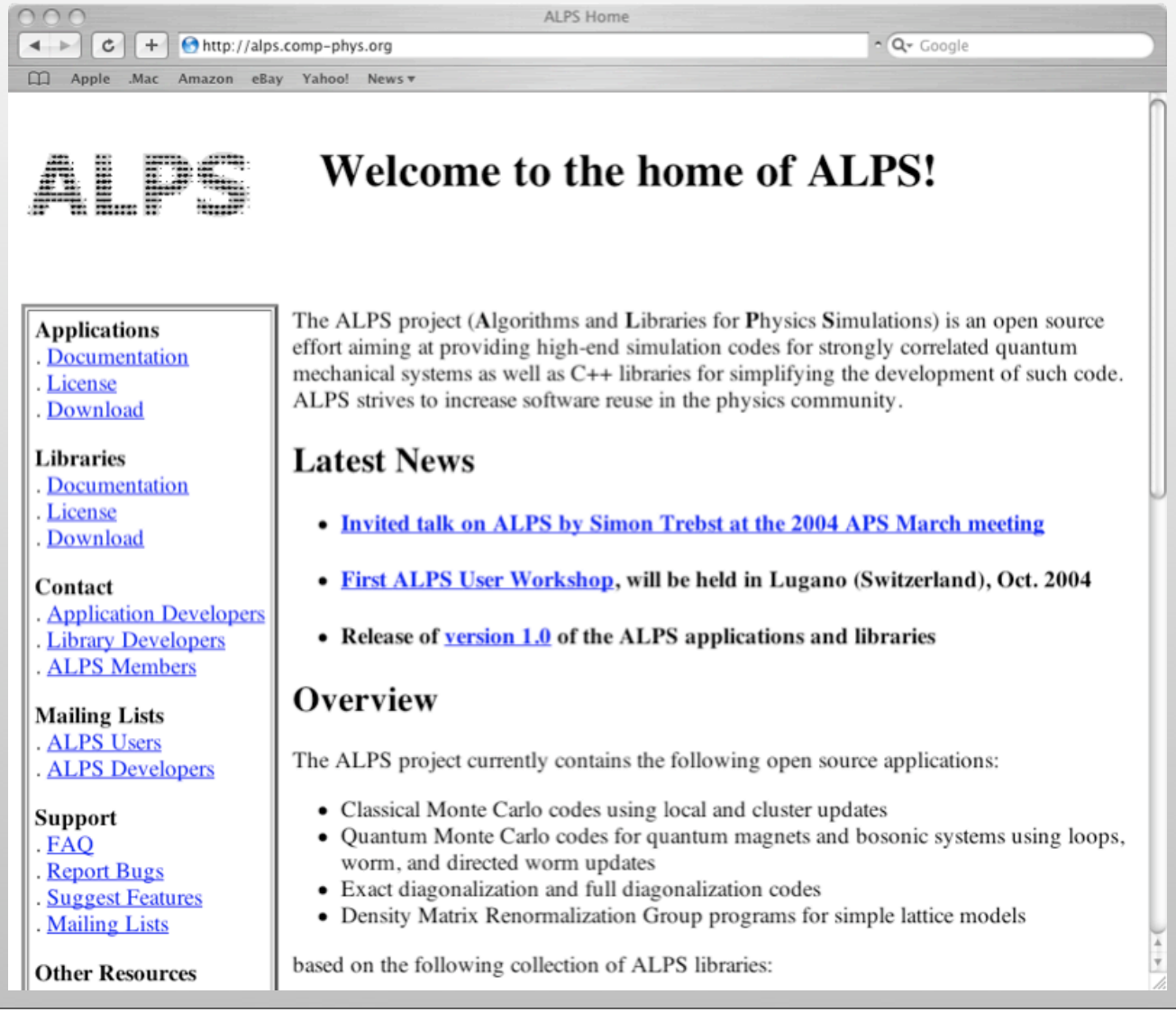
- **Applications codes**
  - free for non-commercial applications
  - based on GNU public license
  - citation requirements
- **Library codes**
  - less restrictive
  - partially available under a free license

User workshops

- **Oak Ridge '03**
  - part of workshop on Wang-Landau sampling
- **Lugano '04**
  - general lectures on numerical methods
  - hands-on tutorials of applications
  - direct feedback from users
  - workshops/tutorials set deadlines for developments

http://alps.comp-phys.org

Become a user yourself!



Funding situation

- Software development classified as **infrastructure project**

  ➡ no funding by research grants

  - combination with research projects
  - no professional code developers

Funding situation

- **Funding sources for infrastructure**
  - computer centers,

    Swiss National Supercomputer Center

    ORNL

  - companies?
  - think big: group grant

    can fund a software developer
  - open source development helpful

Experiences

- Advantages of open source development ☺
  - improved code design
  - more flexibility
  - code review by fellow developers
- new collaborations, joint research projects ☺
- new contacts to experimental groups ☺
- more work ☹

ALPS workshop '04

Lugano, September 26 - October 1

Invited speakers

F. Alet
G. Brown
H.-G. Evertz
C. Kollath
A. Läuchli
I. McCulloch
R. Noack
T. Schulthess
S. Todo
S. Trebst
Shan-Ho Tsai

Hands-on tutorials

Classical Monte Carlo
Spin Dynamics
Quantum Monte Carlo
Exact diagonalization
DMRG