Get the most of now!

Jürgen Schnack

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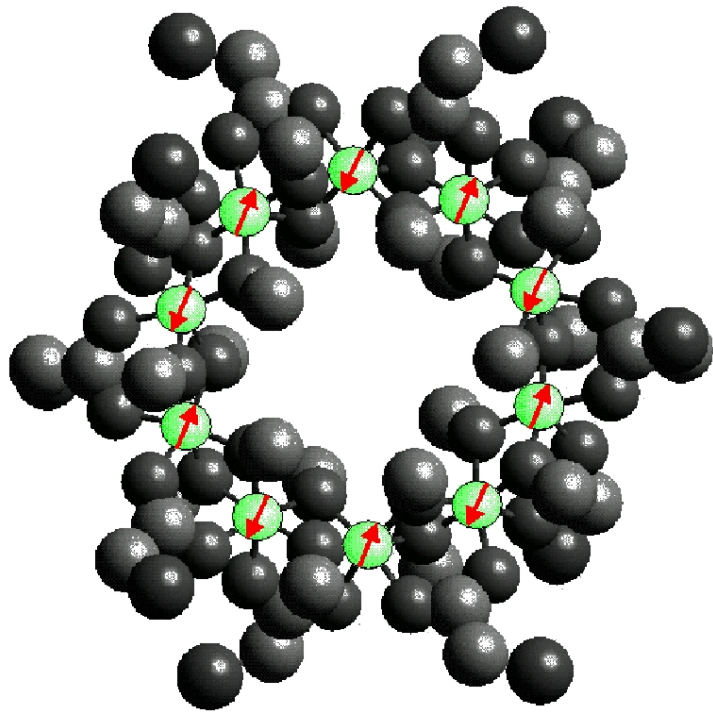
http://obelix.physik.uni-bielefeld.de/$\sim$schnack/

Dedication of the Bielefeld HPC

Bielefeld University, June 17, 2010

Universität Bielefeld

DFG

FOR 945
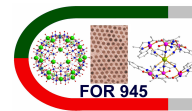
The Leverhulme Trust

Contents for you today
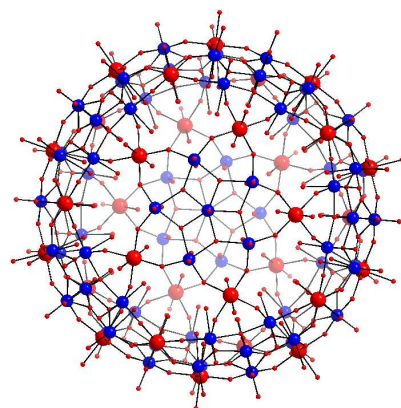

Fe$_{10}$

1. Why?
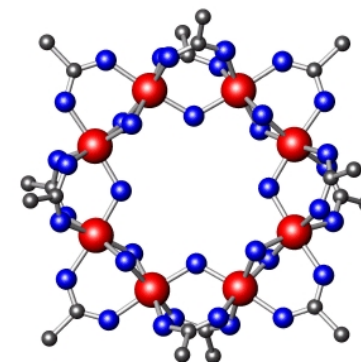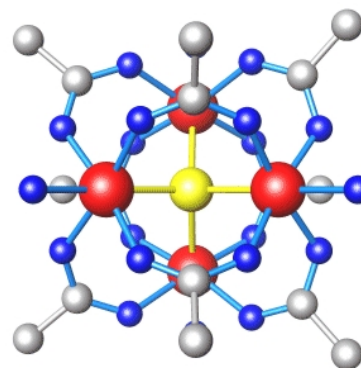
2. How?
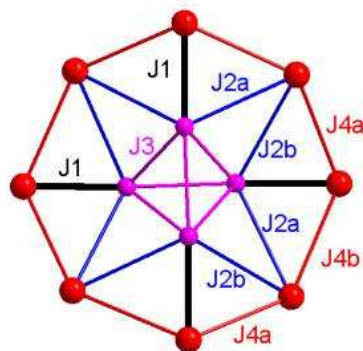
3. Now?

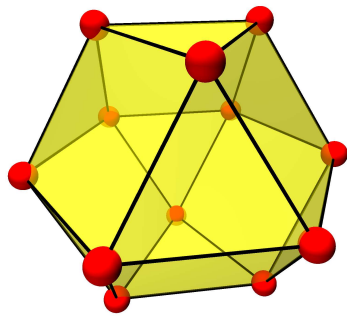4. Wow!

Why?

Magnetic Molecules
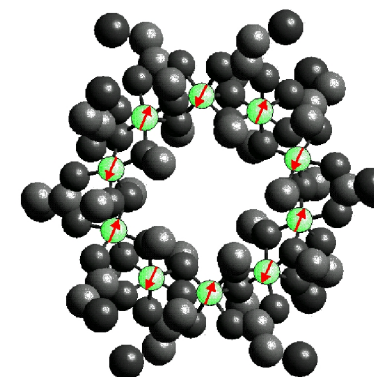
Properties & Function

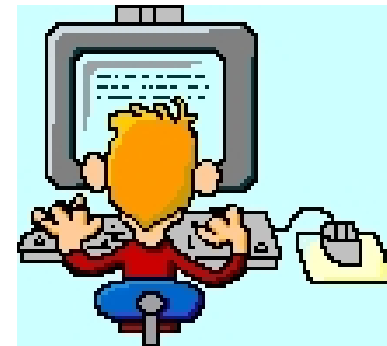# In the end it's always a big matrix!

$$\Rightarrow \begin{pmatrix} -27.8 & 3.46 & 0.18 & \cdots \\ 3.46 & -2.35 & -1.7 & \cdots \\ 0.18 & -1.7 & 5.64 & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{pmatrix} \Rightarrow$$

Isotropic Heisenberg Model
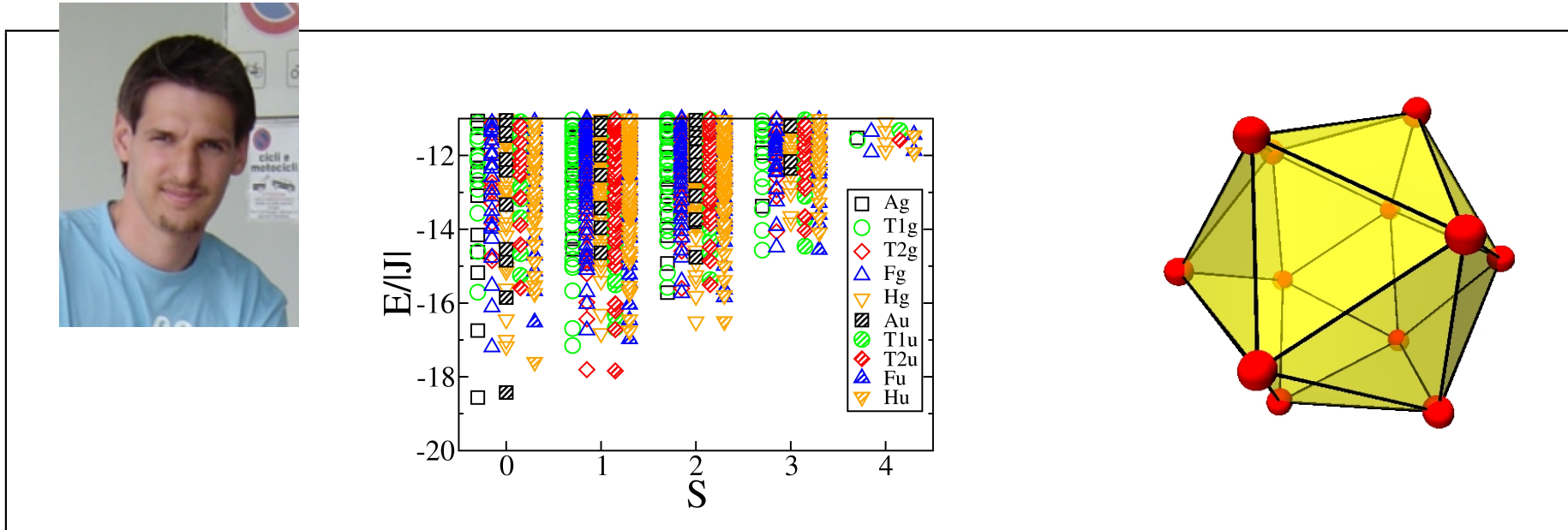
- Exact quantum properties of frustrated spin systems; use of symmetries.

- Elaborate and time-consuming construction of matrices.

- Dr. Roman Schnalle.

Anisotropic Spin Models
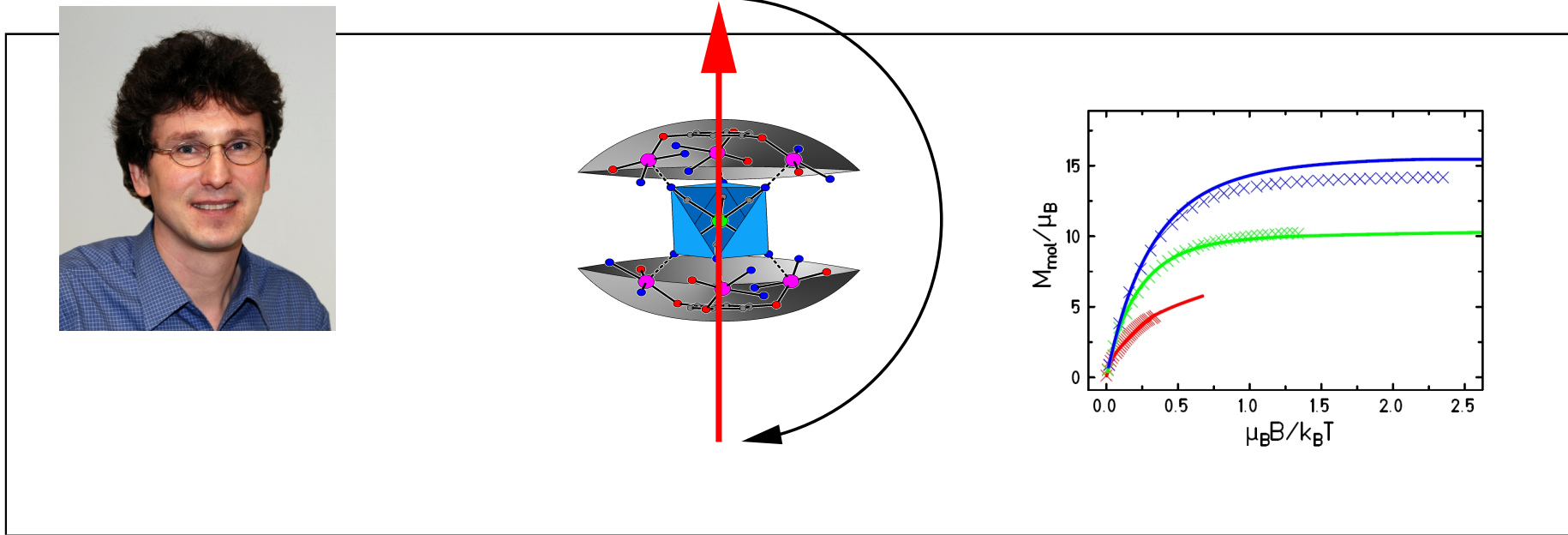
- Search for good Single Molecule Magnets; Complete quantum modelling.

- Search among hundreds of big matrices to find appropriate model.

- Jürgen Schnack, FOR 945

Density Matrix Renormalization Group technique

1,073,741,824
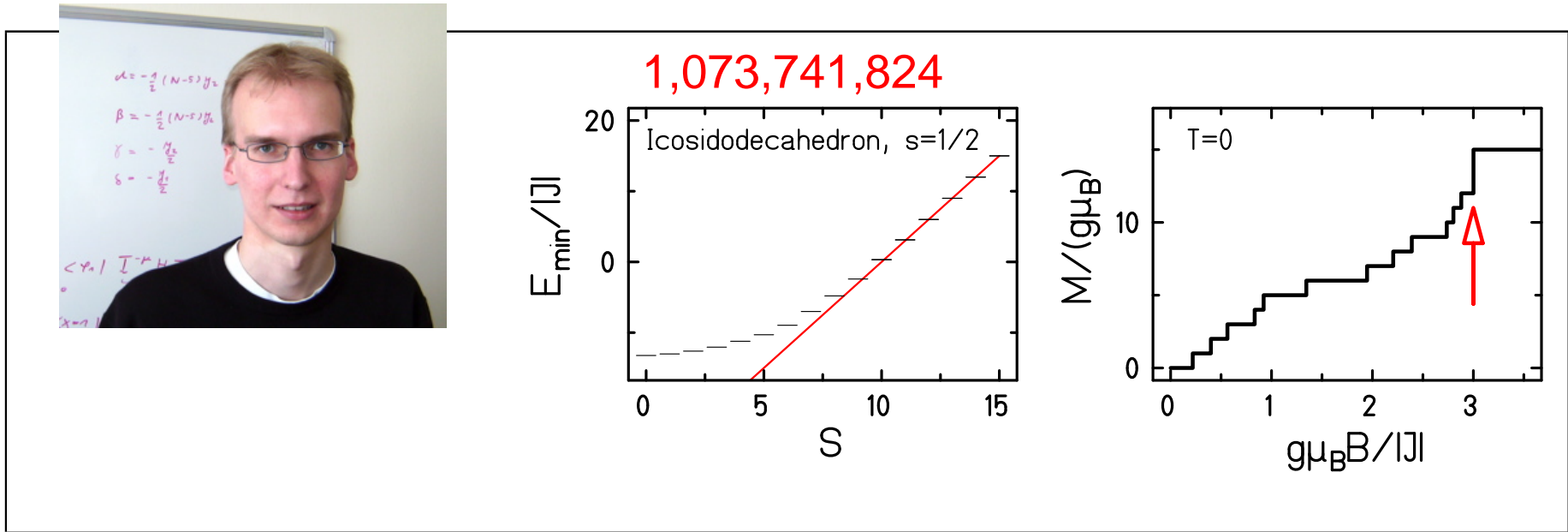
- Approximate calculation of magnetic properties.

- 221,073,919,720,733,357,899,776 (0.2 Quadrillion, l.s.c.)

- Ph. D. project Jörg Ummethum.
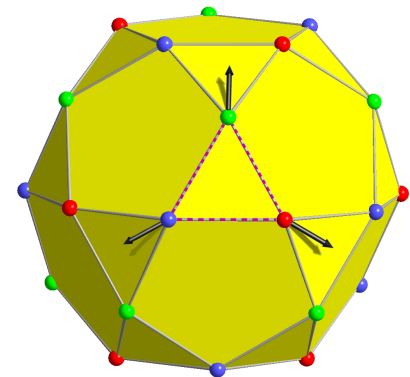
Hubbard model and Numerical Renormalization Group calculations
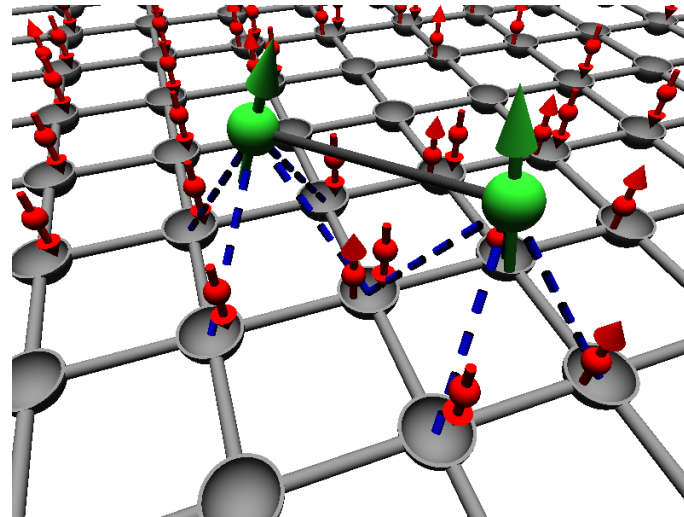
- FOR 945: Investigation of deposited magnetic clusters.

- NRG: Approximation of the infinite system by a sequence of matrices.

- Ph. D. project Martin Höck.

Density Functional Theory calculations
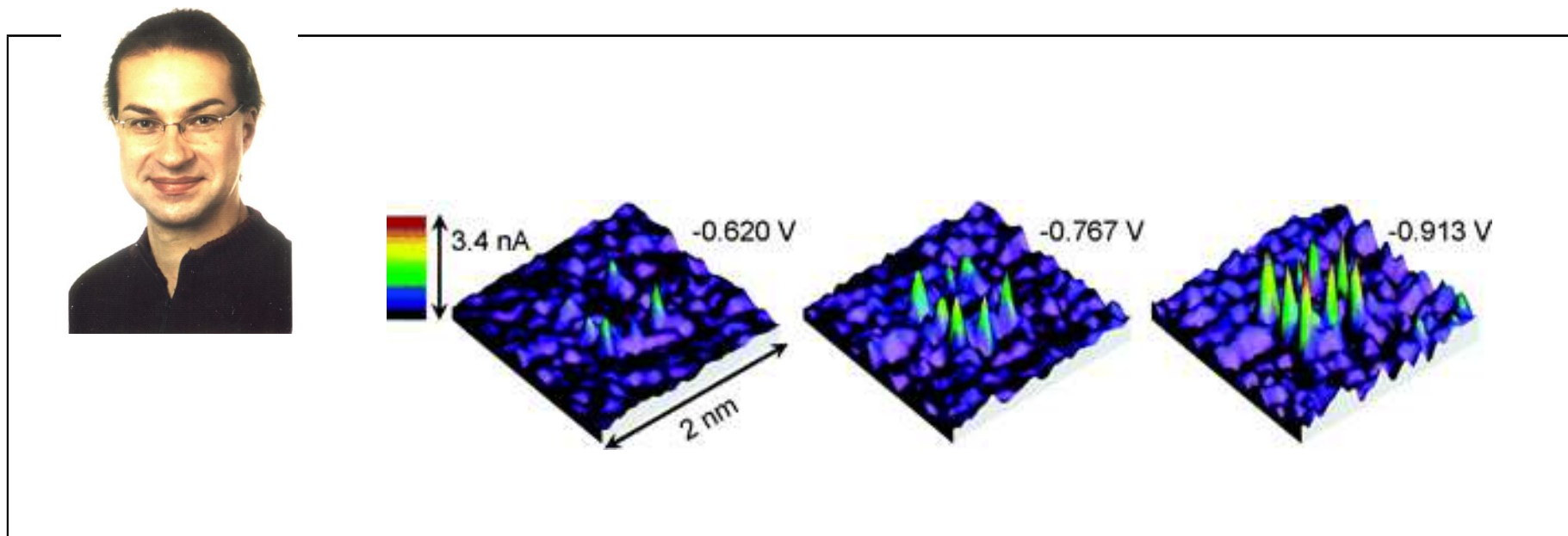
- DFT calculations for polyoxometalates;

- FOR 945: DFT calculations for molecules $M_6^t M^c$ from the Glaser group;

- Prof. Andrei Postnikov (Metz) & Ph. D. project Stefan Leiding.

How?

brain power

&

computing power

How II – BULL and ScaleMP
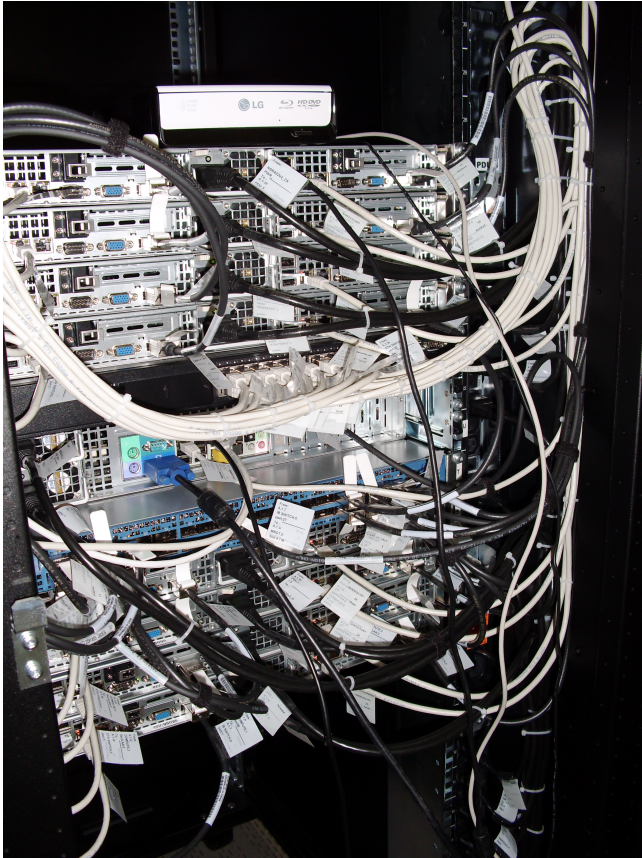
- 16 boards

- 2 Quad Nehalem + $2 \times 3 \times 4$ GB RAM per board

- IB, QDR

- login node

- up and running 24h per day

Now?

Now I – business as usual


```
schnack@multiplet02:~/hpc/Icosahedron

File   Edit   View   Terminal   Tabs   Help

top - 16:39:20 up 50 days,  7:51,  1 user,  load average: 66.32, 50.26, 27.63
Tasks: 1464 total,   3 running, 1461 sleeping,   0 stopped,   0 zombie
Cpu(s): 50.7%us,  0.0%sy,  0.0%ni, 48.9%id,  0.0%wa,  0.0%hi,  0.4%si,  0.0%st
Mem:  329857828k total, 64431536k used, 265426292k free,   154296k buffers
Swap:  5116692k total,        0k used,  5116692k free,  4723000k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
13575 schnack   25   0 18.0g  17g 3592 R 5705.4  5.6 357:05.80 tlanczos-15-ico
18221 rschnall  25   0 37.2g  36g 4728 R 800.0 11.5 201392:45 transmainM
13669 schnack   16   0 13796 2168  808 R  4.5  0.0   0:05.28 top
    1 root      18   0 10352  700  588 S  0.0  0.0  17:17.67 init
    2 root      RT   0     0    0    0 S  0.0  0.0   0:00.67 migration/0
    3 root      34  19     0    0    0 S  0.0  0.0   0:05.18 ksoftirqd/0
    4 root      RT   0     0    0    0 S  0.0  0.0  13:43.05 watchdog/0
    5 root      RT   0     0    0    0 S  0.0  0.0   0:00.37 migration/1
    6 root      34  19     0    0    0 S  0.0  0.0   0:18.29 ksoftirqd/1
    7 root      RT   0     0    0    0 S  0.0  0.0   2:42.46 watchdog/1
```
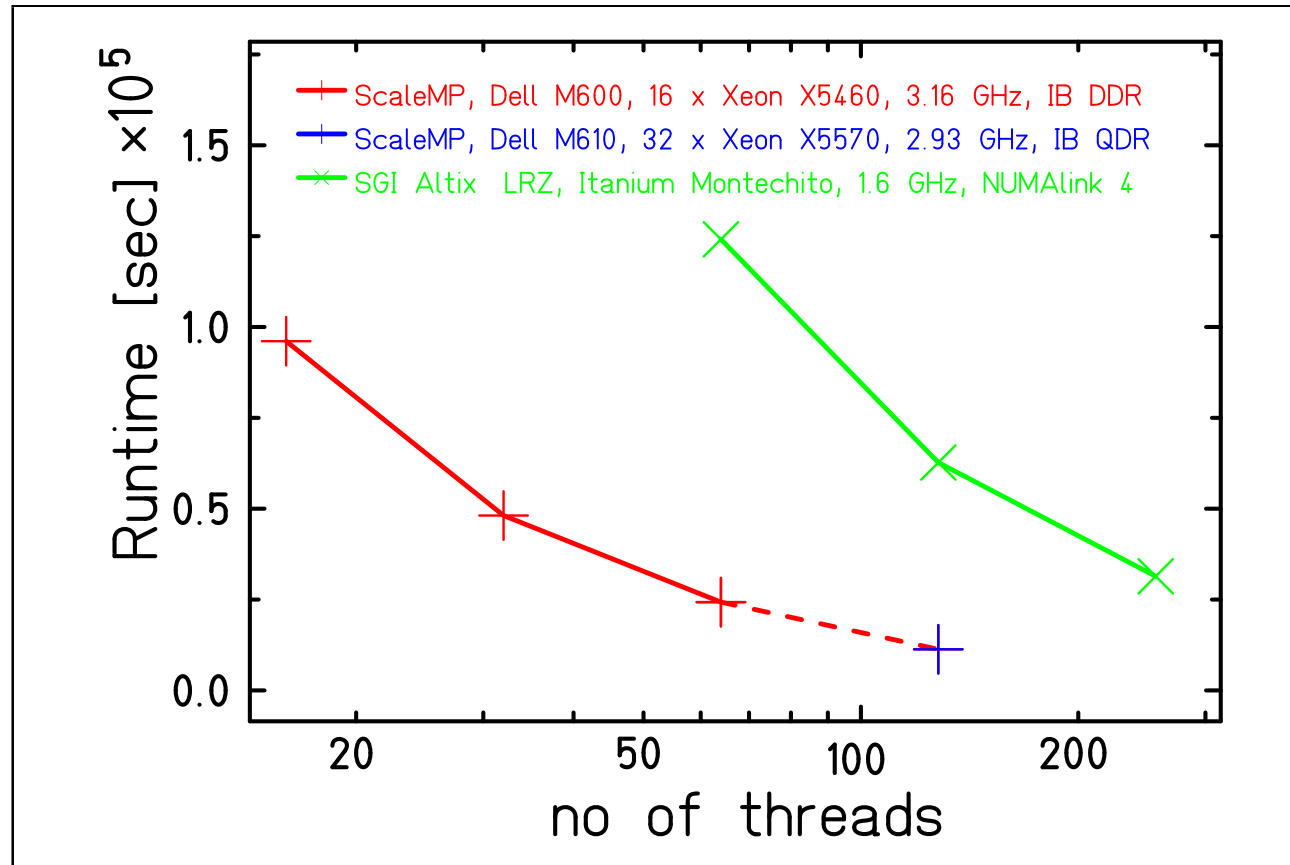
Several jobs running, e.g. Lanczos on 64 cores by `schnack` and complete matrix diagonalizations on 8 cores by `rschnall`.
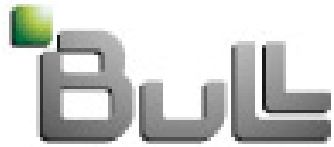
Now II – Lanczos scaling

Almost perfect scaling of openMP parallelized Lanczos code: the SGI Altix (LRZ) is compared to new DELL machines using ScaleMP. The dimension of the underlying Hilbert space, i.e. the length of the used Lanczos vectors is 601,080,390.

Wow!

Many thanks

- Many thanks to BULL and ScaleMP for very good consultations when ordering, installing, and experiencing *childhood* problems.

- Many thanks to Bielefeld University for supporting this machine and for the very professional way to get it to Bielefeld.

- Many thanks to my group for the research enthusiasm, which is always necessary to milk scientific progress from the hardware. It helps if the latter is outstanding.

2008

2010

Thank you very much for your attention.

Molecular Magnetism Web

www.molmag.de

Highlights.   Tutorials.   Who is who.   Conferences.