Quantenstatistik mit Supercomputern

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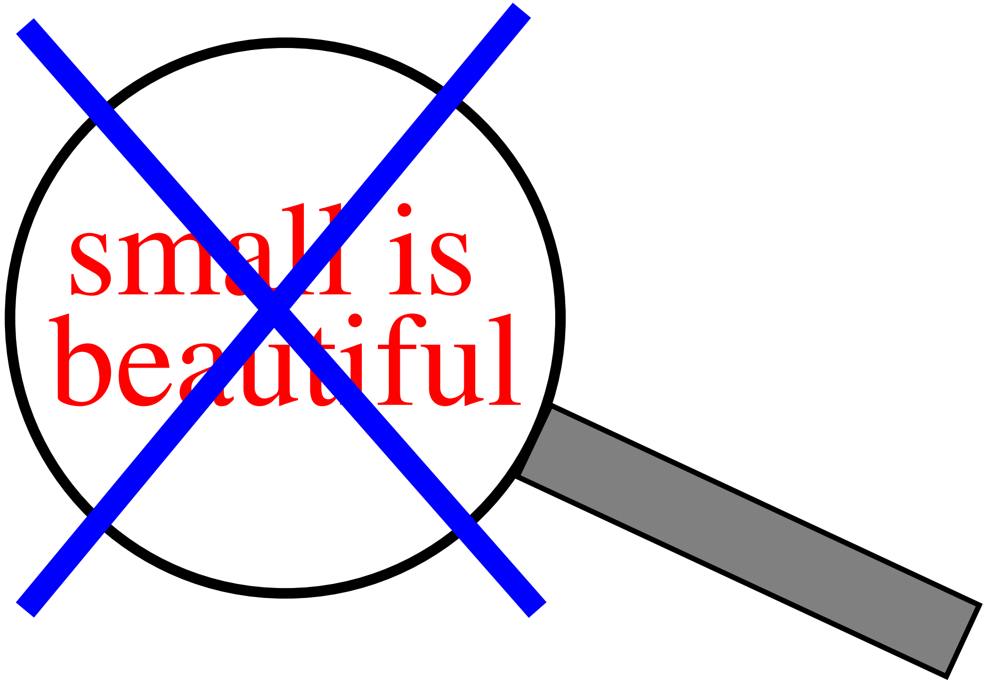
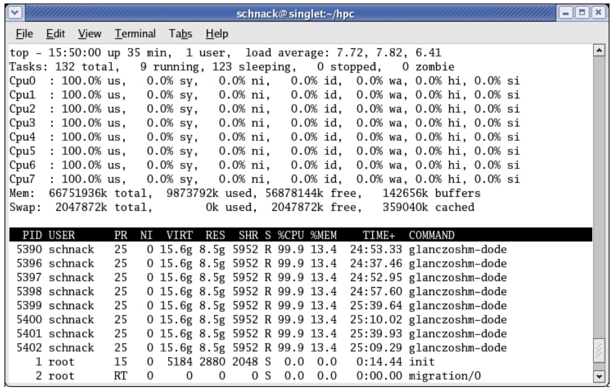
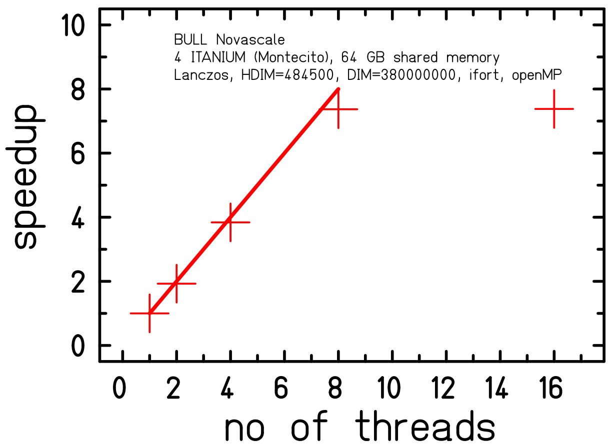
small is
beautiful


~~small is beautiful~~

Size matters!

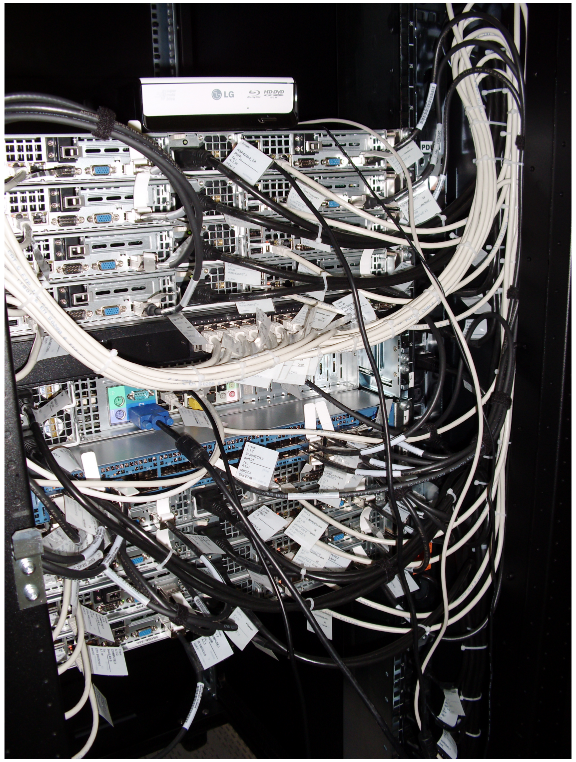
Osnabrück anno 2001





BULL: 4 Itanium dual core, 64 GB RAM

Bielefeld anno 2009



BULL: 16 nodes, 2 INTEL quadcore CPUs/node, 386 GB RAM, vSMP

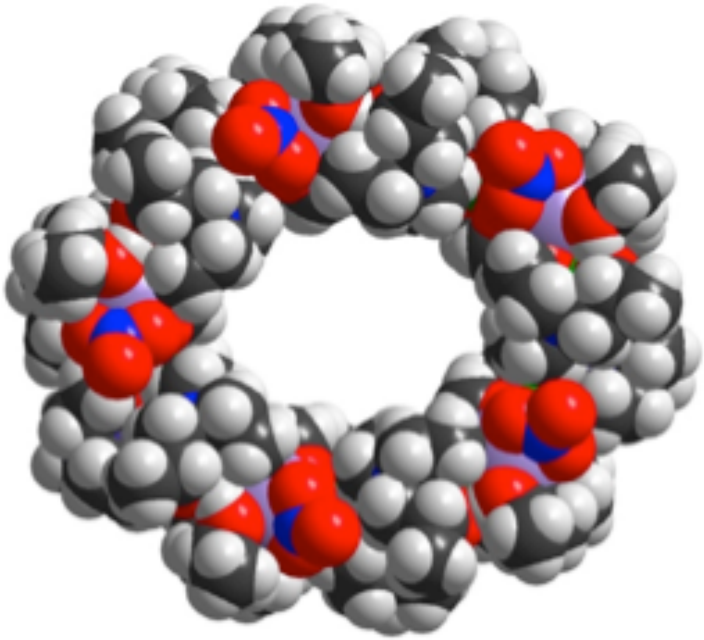
Garching anno 2012

Supercomputer **SuperMUC** am Leibniz-Rechenzentrum in Garching:
3 PFLOPS/s, mehr als 150,000 Intel-Prozessor-Cores (Xeon E5)

And now Osnabrück again!

But why HPC?

You have got a molecule!

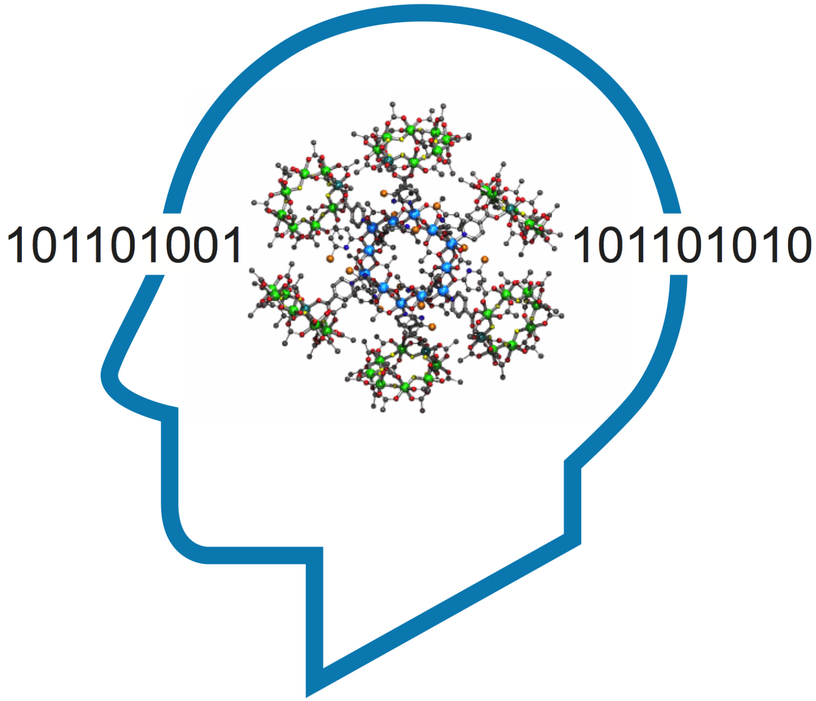


$$S = 60!$$

Congratulations!

Powell group: npj Quantum Materials **3**, 10 (2018)

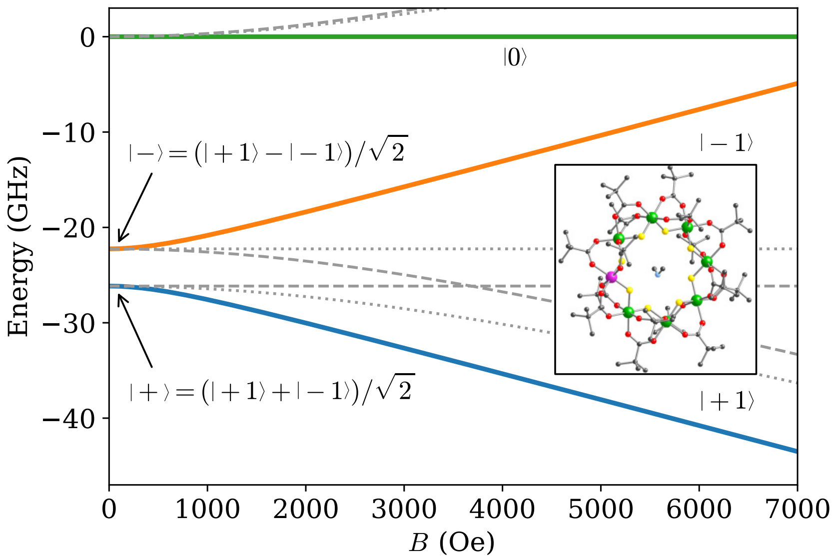
You want to build a quantum computer!



Very smart!

Wernsdorfer group: Phys. Rev. Lett. **119**, 187702 (2017)

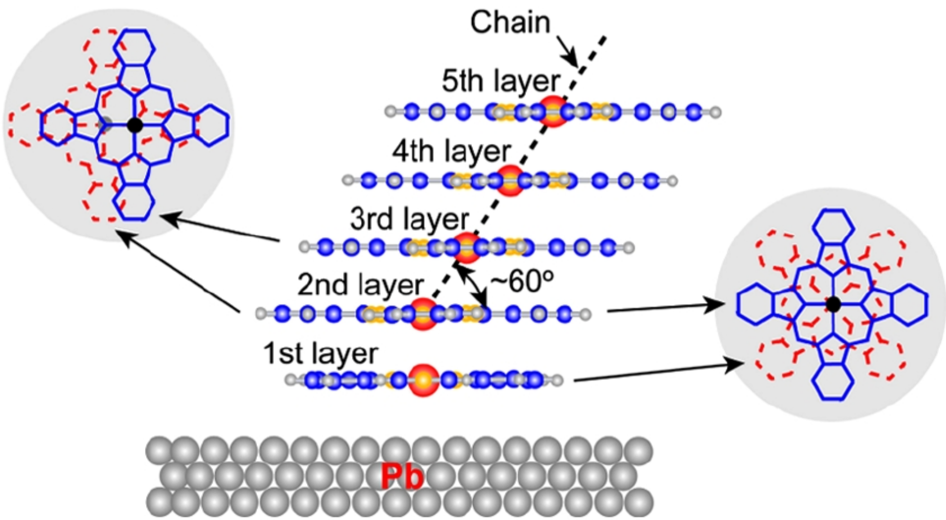
You want to achieve quantum coherence!



Desperately needed!

Friedman group: Phys. Rev. Research **2**, 032037(R) (2020)

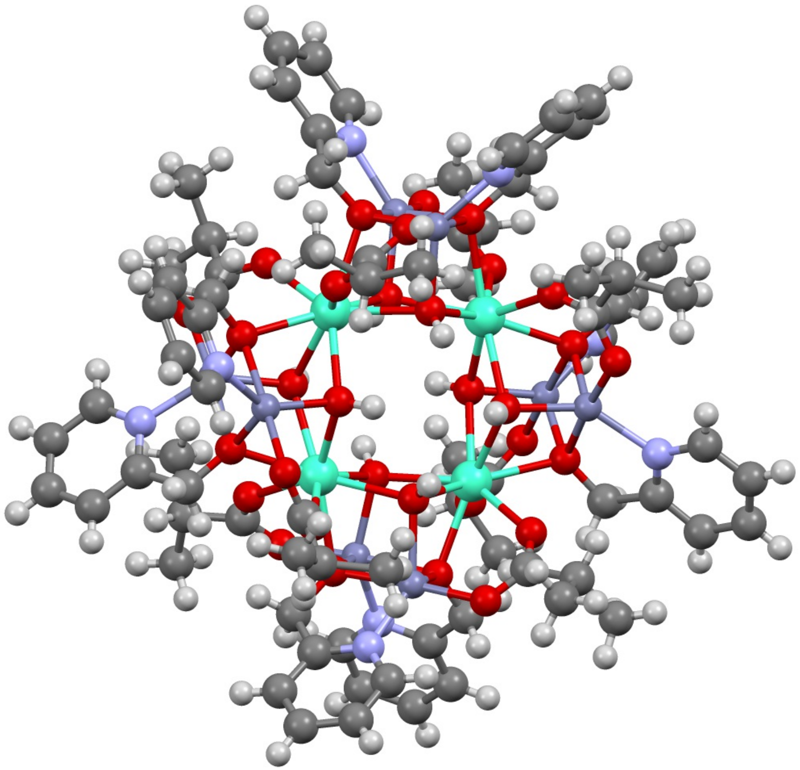
You want to deposit your molecule!



Next generation magnetic storage!

Xue group: Phys. Rev. Lett. **101**, 197208 (2008)

You want molecular magnetocalorics!



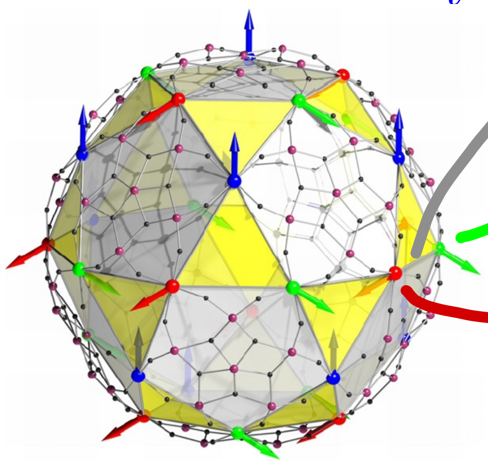
Cool!

Brechin group: Angew. Chem. Int. Ed. **51**, 4633 (2012)

You have got an idea about the modeling!

Heisenberg **Zeeman**

$$\underset{\sim}{H} \;=\; -2\sum_{i<j} J_{ij}\,\underset{\sim}{\vec{s}}(i)\cdot\underset{\sim}{\vec{s}}(j) + g\,\mu_B\,B\sum_{i}^{N}\underset{\sim}{s}_z(i)$$



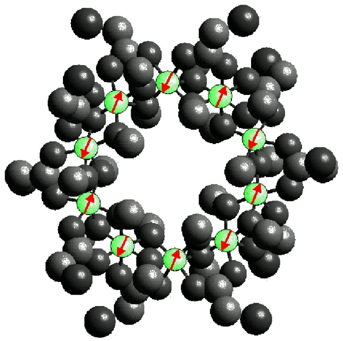
You have to solve the Schrödinger equation!

$$\underset{\sim}{H} \mid \phi_n \rangle = E_n \mid \phi_n \rangle$$

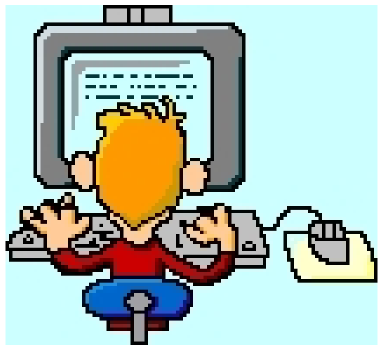
Eigenvalues E_n and eigenvectors $\mid \phi_n \rangle$

- needed for spectroscopy (EPR, INS, NMR);
- needed for thermodynamic functions (magnetization, susceptibility, heat capacity);
- needed for time evolution (pulsed EPR, simulate quantum computing, thermalization).

In the end it's always a big matrix!



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



Fe$^{\mathrm{III}}_{10}$: $N = 10$, $s = 5/2$, dim$(\mathcal{H}) = (2s+1)^N$

Dimension=60,466,176. Maybe too big?

Can we evaluate the partition function

$$Z(T,B) = \text{tr}\left(\exp\left[-\beta \underset{\sim}{H}\right]\right)$$

without diagonalizing the Hamiltonian?

Yes, with magic!

Quantum statistics with HPC

(Magic + Power)

Solution I: trace estimators

$$\text{tr}\left(\underset{\sim}{O}\right) \approx \langle\, r \,|\, \underset{\sim}{O} \,|\, r \,\rangle = \sum_{\nu} \langle\, \nu \,|\, \underset{\sim}{O} \,|\, \nu \,\rangle + \sum_{\nu \neq \mu} r_\nu r_\mu \langle\, \nu \,|\, \underset{\sim}{O} \,|\, \mu \,\rangle$$

$$|\, r \,\rangle = \sum_{\nu} r_\nu \,|\, \nu \,\rangle \,, \quad r_\nu = \pm 1$$

- $|\, \nu \,\rangle$ some orthonormal basis of your choice;
  not the eigenbasis of $\underset{\sim}{O}$, since we don't know it.
- $r_\nu = \pm 1$ random, equally distributed. Rademacher vectors.
- Amazingly accurate, bigger (Hilbert space dimension) is better.

M. Hutchinson, Communications in Statistics - Simulation and Computation **18**, 1059 (1989).

Solution II: Krylov space representation

$$\exp\left[-\beta \underset{\sim}{H}\right] \approx \underset{\sim}{1} - \beta \underset{\sim}{H} + \frac{\beta^2}{2!}\underset{\sim}{H}^2 - \dots \frac{\beta^{N_L-1}}{(N_L-1)!}\underset{\sim}{H}^{N_L-1}$$

applied to a state $\mid r \,\rangle$ yields a superposition of

$$\underset{\sim}{1} \mid r \,\rangle, \quad \underset{\sim}{H} \mid r \,\rangle, \quad \underset{\sim}{H}^2 \mid r \,\rangle, \quad \dots \underset{\sim}{H}^{N_L-1} \mid r \,\rangle \ .$$

These (linearly independent) vectors span a small space of dimension N_L;
it is called Krylov space.

Let's diagonalize $\underset{\sim}{H}$ in this space!

Partition function I: simple approximation

$$Z(T,B) \approx \langle\, r \,|\, e^{-\beta \underset{\sim}{H}} \,|\, r \,\rangle \approx \sum_{n=1}^{N_L} e^{-\beta \epsilon_n^{(r)}} |\langle\, n(r) \,|\, r \,\rangle|^2$$

$$O^{\mathrm{r}}(T,B) \approx \frac{\langle\, r \,|\, \underset{\sim}{O} e^{-\beta \underset{\sim}{H}} \,|\, r \,\rangle}{\langle\, r \,|\, e^{-\beta \underset{\sim}{H}} \,|\, r \,\rangle} = \frac{\langle\, r \,|\, e^{-\beta \underset{\sim}{H}/2} \underset{\sim}{O} e^{-\beta \underset{\sim}{H}/2} \,|\, r \,\rangle}{\langle\, r \,|\, e^{-\beta \underset{\sim}{H}/2} e^{-\beta \underset{\sim}{H}/2} \,|\, r \,\rangle}$$

- Wow!!!
- One can replace a trace involving an intractable operator by an expectation value with respect to just ONE random vector evaluated by means of a Krylov space representation???
- Typicality = any random vector will do: $|\, r \,\rangle \equiv (T = \infty)$

J. Jaklic and P. Prelovsek, Phys. Rev. B **49**, 5065 (1994).

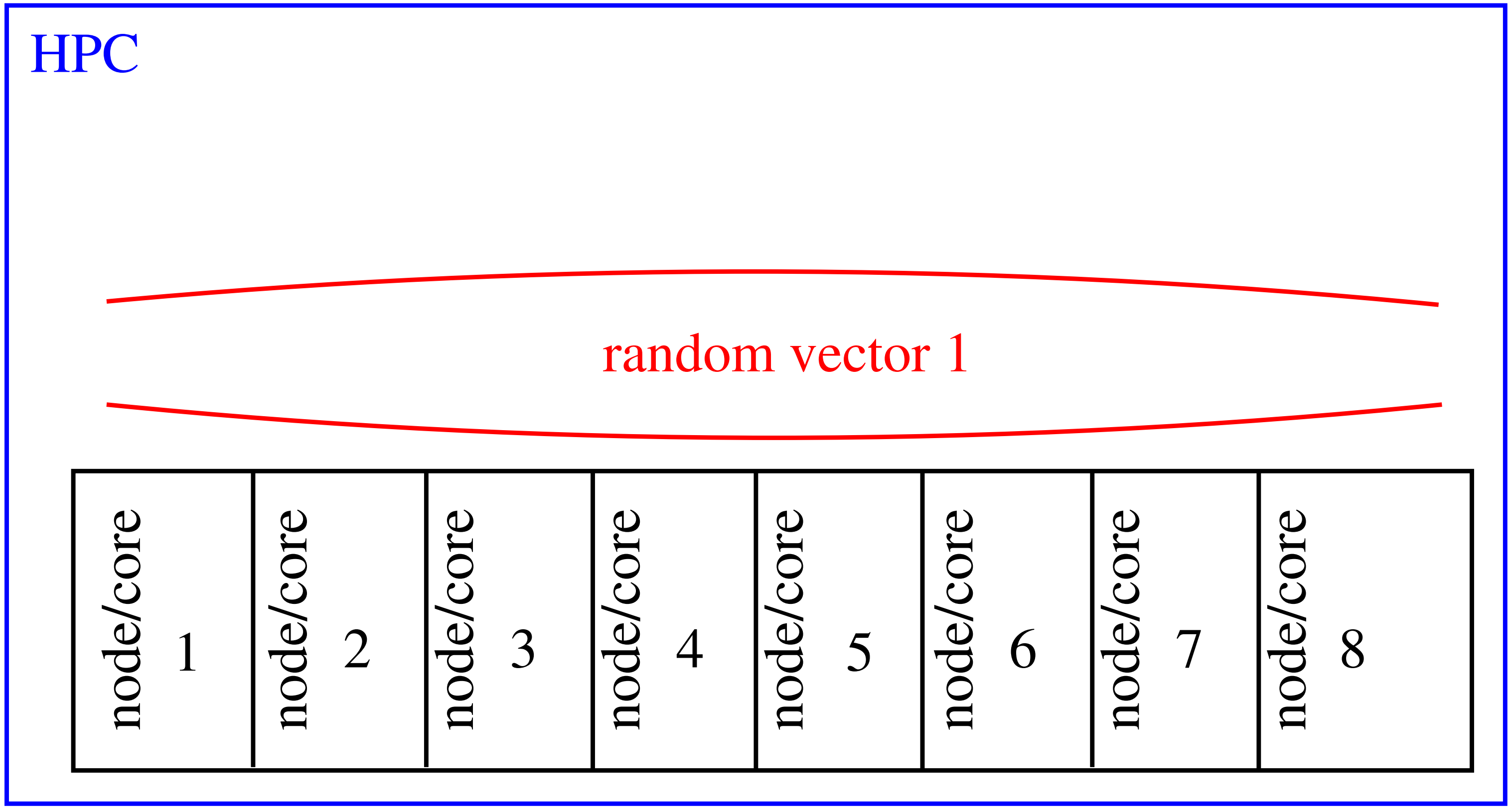
Partition function II: Finite-temperature Lanczos Method

$$Z^{\mathrm{FTLM}}(T,B) \approx \frac{1}{R}\sum_{r=1}^{R}\sum_{n=1}^{N_L} e^{-\beta\epsilon_n^{(r)}} |\langle\, n(r) \,|\, r\,\rangle|^2$$

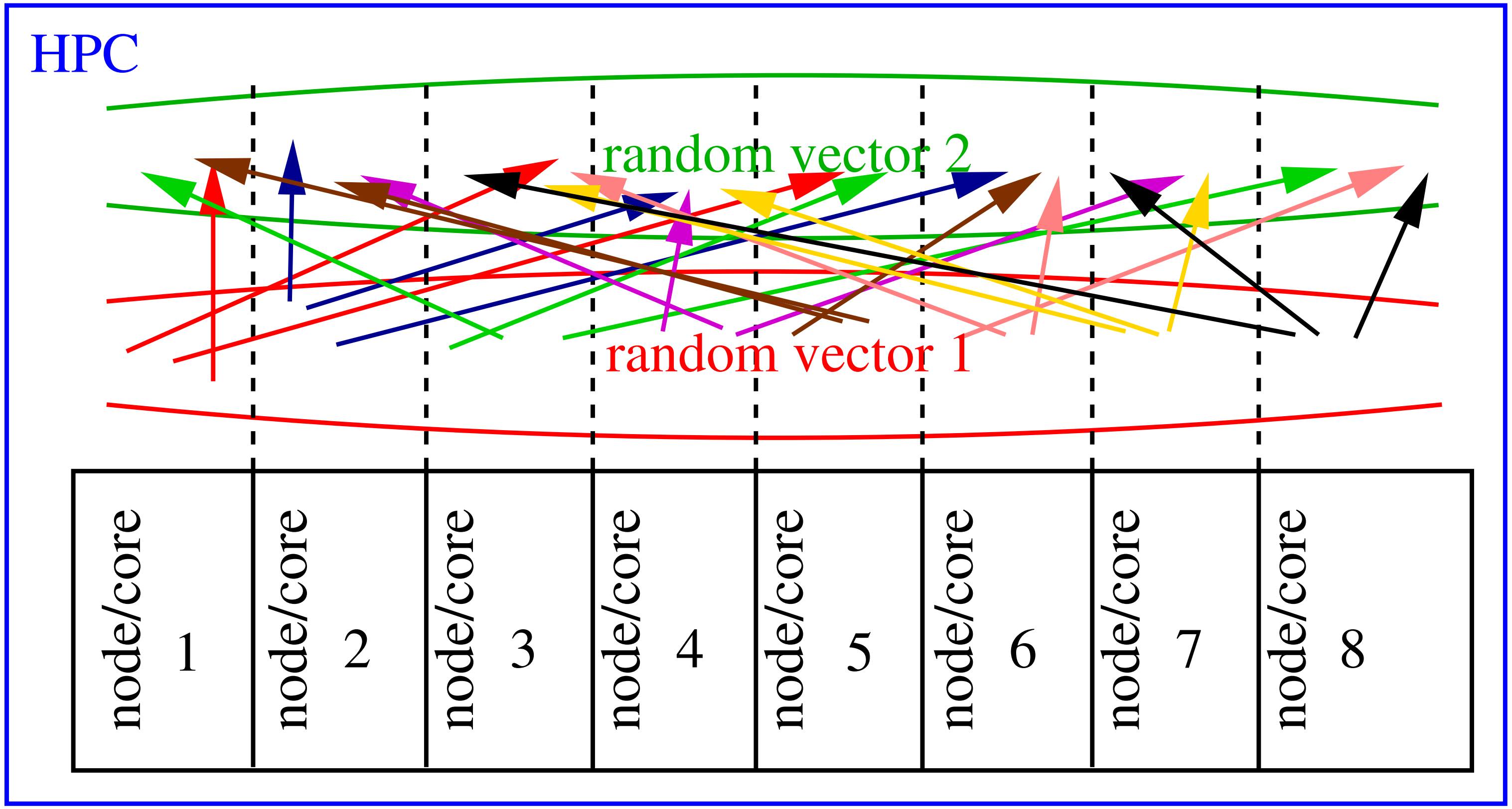
- Averaging over R random vectors is better.
- $|\, n(r)\,\rangle$ n-th Lanczos eigenvector starting from $|\, r\,\rangle$.
- Partition function replaced by a small sum: $R = 1 \dots 100, N_L \approx 100$.
- Implemented in `spinpack` by Jörg Schulenburg (URZ Magdeburg); MPI and openMP parallelized, used up to 3072 nodes.

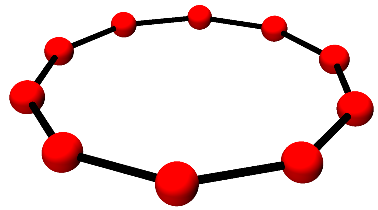
SPINPACK page: https://www-e.uni-magdeburg.de/jschulen/spin/

Matrix vector operations with HPC I

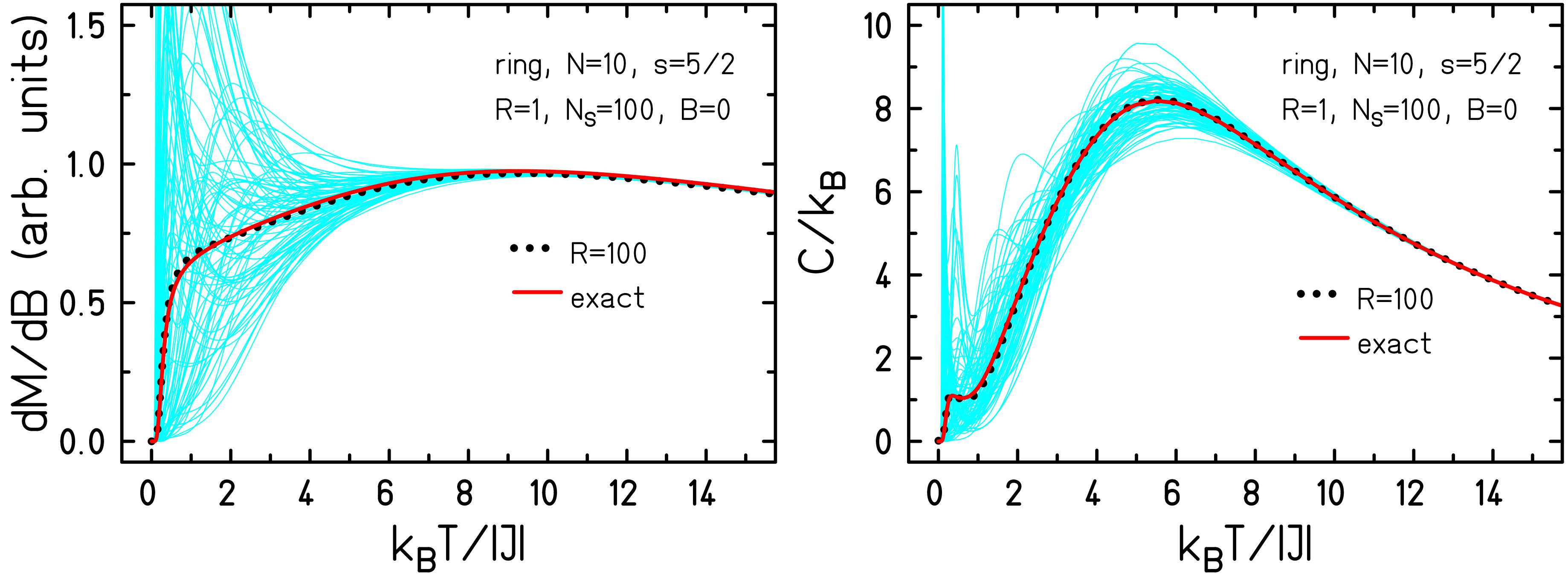


Matrix vector operations with HPC II





FTLM 1: ferric wheel



(1) J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research **2**, 013186 (2020).

(2) SU(2) & D_2: R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29**, 403 (2010).

(3) SU(2) & C_N: T. Heitmann, J. Schnack, Phys. Rev. B **99**, 134405 (2019)

HPC3, go with throttle up!

Molecular Magnetism Web

www.molmag.de

Highlights. Tutorials. Who is who. Conferences.