Optimization through extra dimensions: the Ising spin glass

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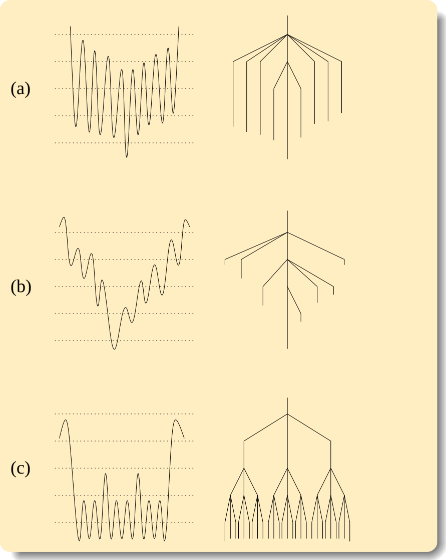
Outline

Metastability and optimization hardness



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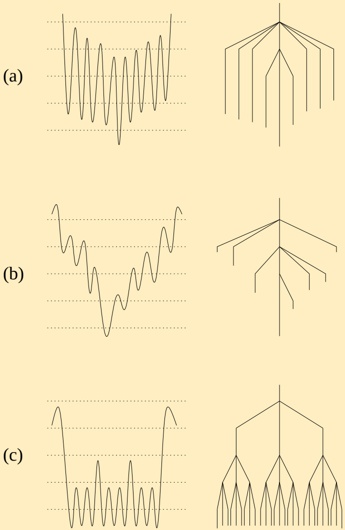

Metastability

Metastability

- is at the heart of many features of complex systems
- is crucial for the understanding of dynamic phenomena
- prevents equilibration in simulations due to diverging time scales
- is related to (NP) hardness of associated optimization (ground state) problems

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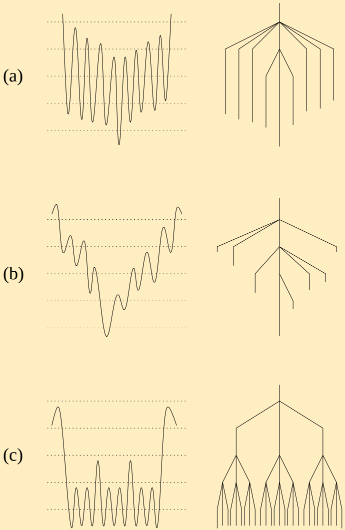

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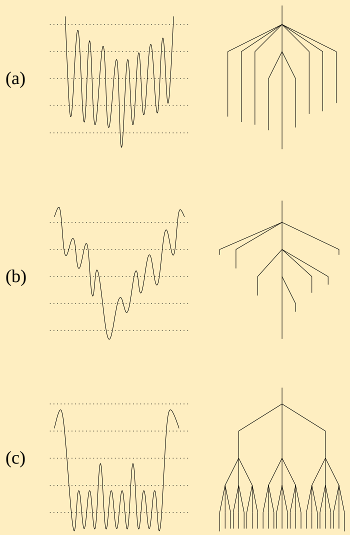

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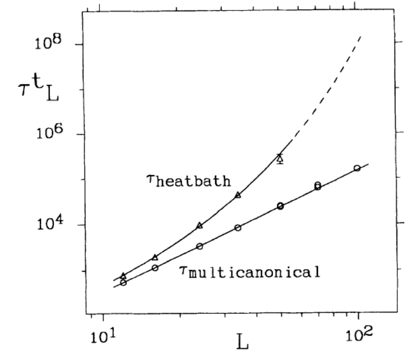
Metastability and optimization hardness

Monte Carlo simulations



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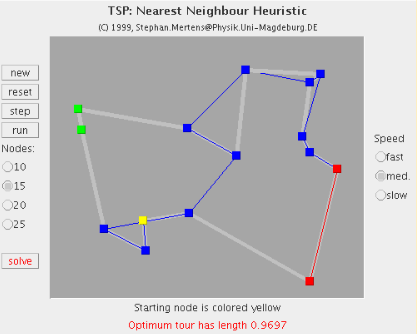
Metastability and optimization hardness

Traveling salesman problem



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Conventional solutions

Techniques

- multicanonical, flat/broad histogram, Wang-Landau simulations
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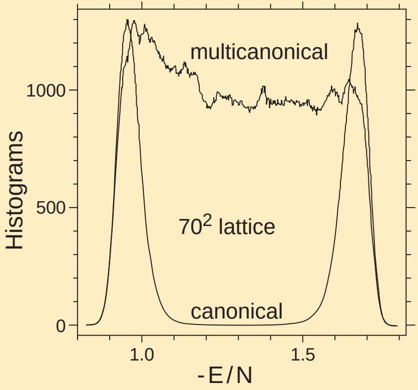

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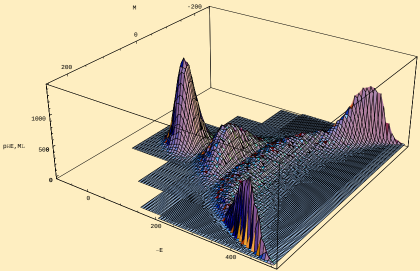

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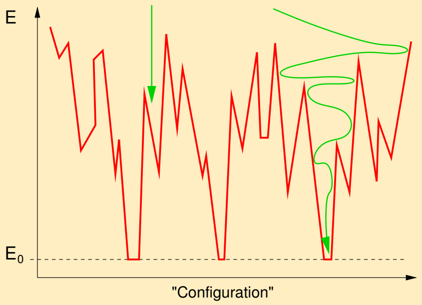

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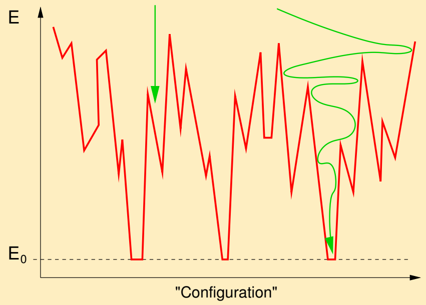

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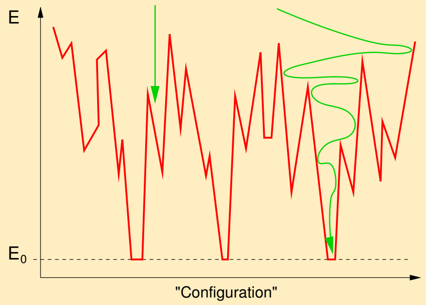

Conventional wisdom: go around or climb above the mountains, or fill up the valleys!

Metastability in particle systems

Consider dynamical system of point particles in D dimensions with pair potentials

$$U_{ij} = -J_{ij}|\boldsymbol{r}_i - \boldsymbol{r}_j|^{\alpha}. \tag{1}$$

Then, stationary points originate in pair potentials ...

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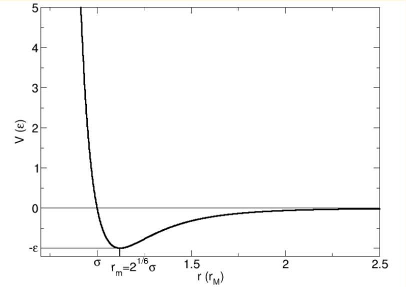

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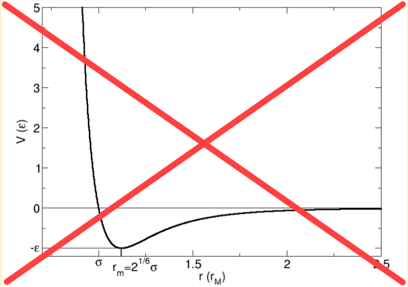

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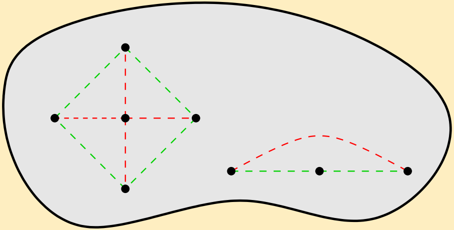

For instance for embedding in a patch of the plane ($D = 2$).

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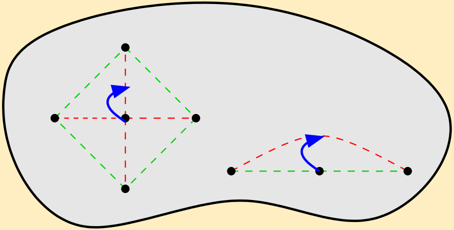

Idea (`Nussinov`[2]`, cond-mat/0209155`): escape to another dimension!

Obviously, for $D = N$, all difference vectors $\boldsymbol{r}_i - \boldsymbol{r}_j$ are linearly independent and no cancellation/metastability can occur.

Lack of metastability in high dimensions

In high dimensions: each state of N particles spans (only) $N-1$ dimensional hyperplane in $\mathbb{R}^D$. This prevents metastability for sufficiently large D.

E.g., for harmonic potential

$$U = -\sum_{i<j} J_{ij}|\boldsymbol{r}_i - \boldsymbol{r}_j|^2 = -\sum_{i<j} J_{ij}(\boldsymbol{r}_i - \boldsymbol{r}_j)\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)^2$$

Metastable state $\{\boldsymbol{r}_i^0\}$, ground state $\{\boldsymbol{r}_i^1\}$, i.e., $E_0 > E_1$. Prepare configurations such that $\boldsymbol{r}_i^0 \cdot \boldsymbol{r}_j^1 = 0\ \forall i \neq j$. Then consider superposition:

$$\boldsymbol{r}_i' = \sqrt{1-\delta^2}\,\boldsymbol{r}_i^0 + \delta\,\boldsymbol{r}_i^1$$

One finds:

$$\left.\frac{\partial U}{\partial \delta}\right|_{\delta=0} = 0$$

$$\left.\frac{\partial^2 U}{\partial \delta^2}\right|_{\delta=0} = -2(E_0 - E_1) < 0$$

Hence, $\boldsymbol{r}^0$ is not metastable! I.e., no metastable states in $D \geq 2(N-1)$.

Representation as minimum-cut problem

Split up Ising model Hamiltonian,

$$-\mathcal{H} = \sum_{\langle ij \rangle} J_{ij}\, s_i s_j = W^+ + W^- - W^\pm = K - 2W^\pm, \tag{2}$$

where $K = \sum_{\langle ij \rangle} J_{ij}$, and

$$W^+ = \sum_{\substack{\langle ij \rangle \\ s_i=s_j=+1}} J_{ij}, \quad W^- = \sum_{\substack{\langle ij \rangle \\ s_i=s_j=-1}} J_{ij}, \quad W^\pm = \sum_{\substack{\langle ij \rangle \\ s_i\neq s_j}} J_{ij} \tag{3}$$

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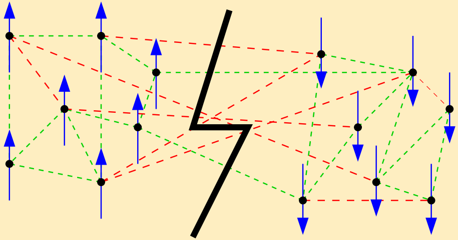

Then, a ground state is given by a configuration with minimal cut $W^\pm$, which divides the spins between the "up" and "down" states.

Auxiliary particle dynamics

Consider dynamical Ising system of point particles with pair potentials

$$U_{ij} = -J_{ij}|\boldsymbol{r}_i - \boldsymbol{r}_j|^\alpha, \tag{4}$$

E.g., for $\alpha = 1$, i.e., constant forces:

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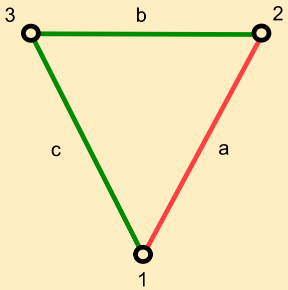

- $E = -a + b + c$
- minimum $E = 0$
- triangle inequality: $a \leq b + c$ with equality only for degenerate triangles

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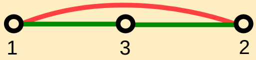

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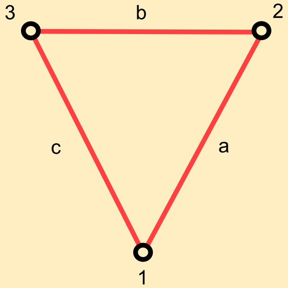

- $E = -a - b - c$
- ground state a, b, $c \to \infty$
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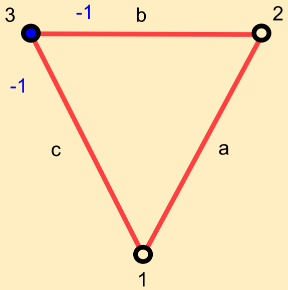

- $E = -a - b - c$
- ground state $a, b, c \to \infty$
- perform Mattis transformation $J_{3j} = -J_{3j}$, $s_3 = -s_3$

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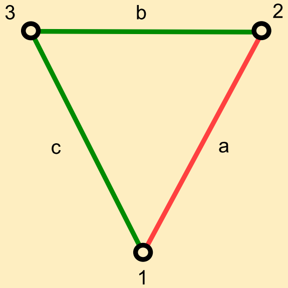
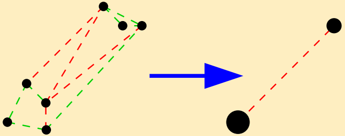


Block spin and Mattis transformations

Block spins

Sequential clustering of spins results in RG-type block spins. Due to high dimension spins do not come close accidentally.



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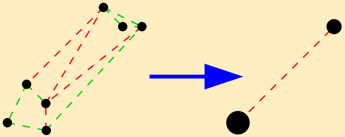
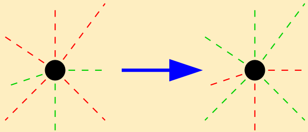


Mattis transformations

For the $\pm J$ model, interactions are overall too repulsive, leading to bad/very slow convergence. Thus, dynamically perform Mattis transformations on (block) spins,



$$\boldsymbol{s}_i \to -\boldsymbol{s}_i, \quad J_{ij} \to -J_{ij} \;\; \forall\, j \,\mathrm{nn}\, i, \qquad (5)$$

to minimise $J_{ij} < 0$. This, however, changes the dynamical system $\Rightarrow$ MSS.

Algorithm

Optimization through extra dimensions

- evolve auxiliary particle system with molecular dynamics simulation:
  - first-order, aristotelian dynamics

$$\boldsymbol{r}_i^{t+1} - \boldsymbol{r}_i^t = \kappa \sum_j \boldsymbol{F}_{ij}$$

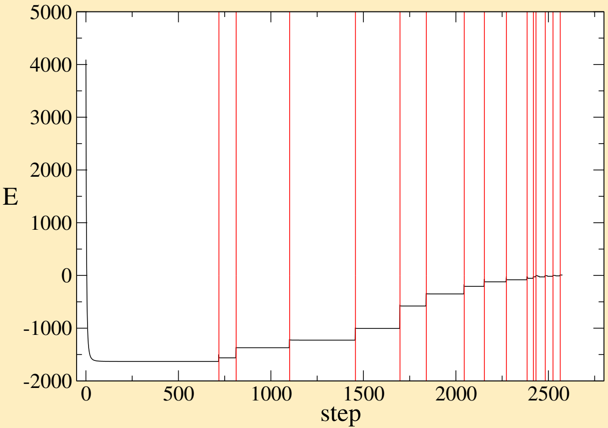
  - or add inertial term: Brownian dynamics, generalized Langevin equation
- force fields/potentials

$$U_{ij} = -J_{ij} |\boldsymbol{r}_i - \boldsymbol{r}_j|^\alpha$$

- embedding dimension: $D = N - 1$ resp. $D = 2(N - 1)$, but in practice much smaller dimension sufficient; $D \propto \sqrt{N}$ sufficient for related problem
- clustering steps for merging vertices
- successive Mattis transformations to reduce repulsiveness

In practice

Energy evolution



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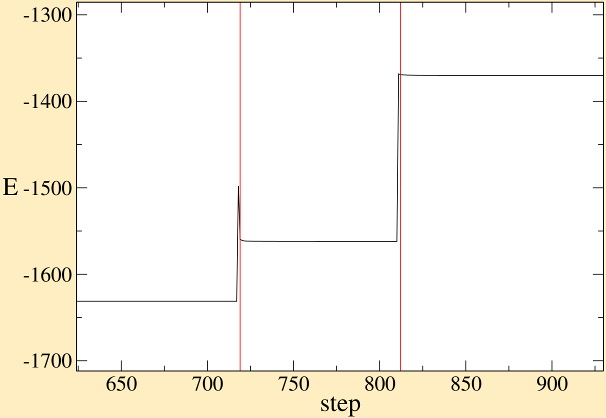

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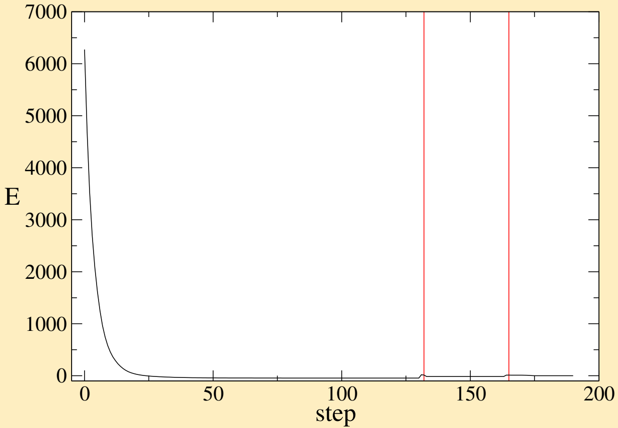
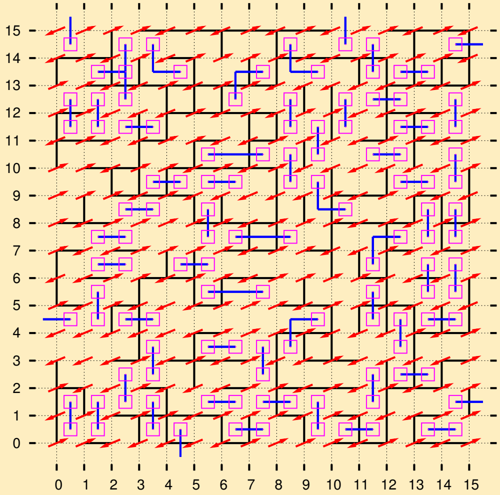


Finds exact ground state of $128 \times 128 \pm J$ samples in $\approx$ 600 s.

In practice

Configurations: effect of Mattis transformations



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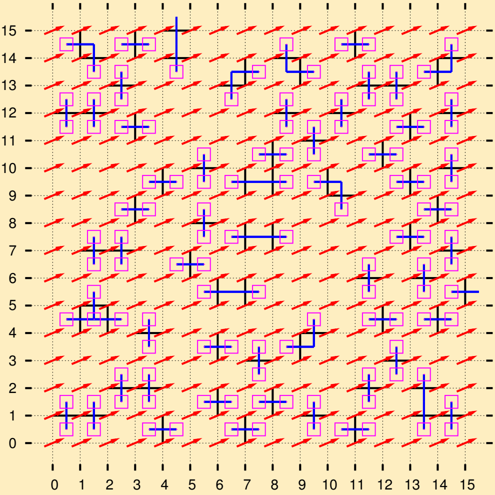

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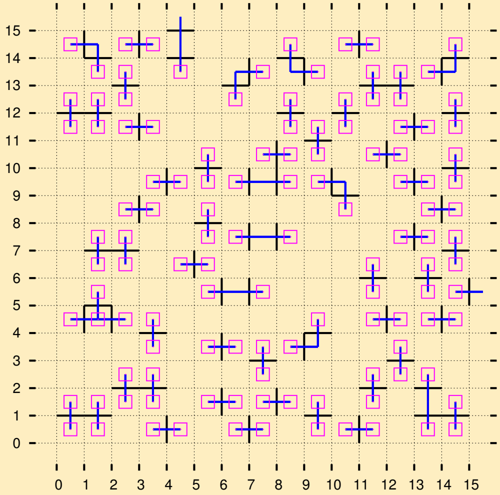
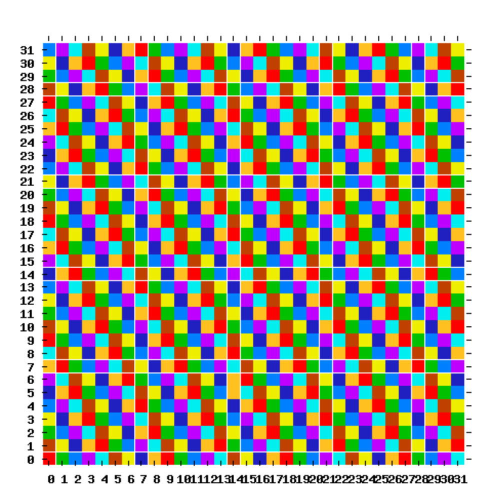


In practice

"Coarsening dynamics"



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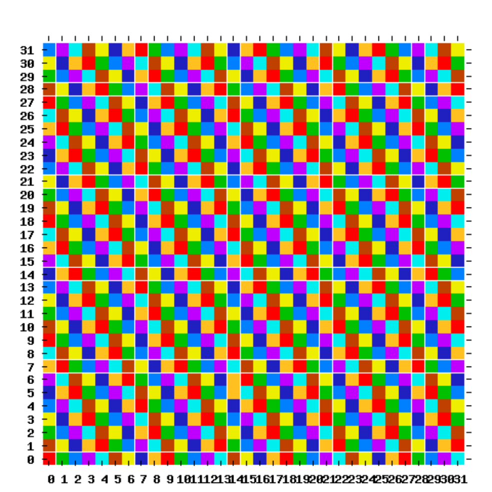

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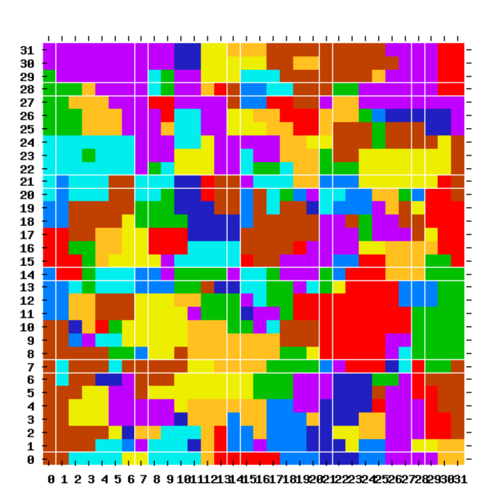

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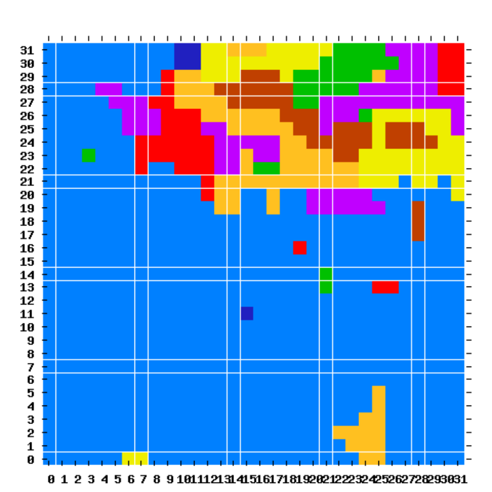

Conclusions

- metastability disappears in high-dimensional extensions of phase space
- this can be exploited to tackle rough energy landscapes in simulation and optimization problems
- auxiliary particle dynamics allows to solve ground-state problem for Ising spin glass for large instances (3D case upcoming)

New Emmy Noether research group

Emmy Noether junior research group on "*Complex systems with frustrating disorder*" to start Jan 1, 2007.

Topics

- spin and structural glasses
- random-field systems
- networks
- ...
- with numerical focus
- closely linked with Binder's group

Positions available for *PhD students* and *postdocs*, please contact me at

weigel@uni-mainz.de

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