Increasing the Efficiency of Physical Optimization Algorithms

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Overview of Optimization Algorithms

- Exact Algorithms
  - Simplex algorithm
    linear cost function, constraints given as inequalities
  - Branch&Bound
    intelligent search with upper and lower bounds
  - Branch&Cut
    solves problems iteratively by adding further cutting planes or performing branching steps

- Heuristic Algorithms
  - Construction Heuristics
    * starting from a Tabula Rasa (e.g., Bestinsertion)
    * starting from an extended system (e.g., Savings)
  - Improvement Heuristics
    * Simulated Annealing
    * Genetic Algorithms
    * Tabu Search
    * Guided Local Search
    * Ant Colony Optimization

Introduction in Physical Optimization Algorithms

Classic Algorithm:

Simulated Annealing

Ingredients:

- Boltzmann Distribution (problem = classic physical system)

$$p(\sigma) = \frac{1}{Z} \exp\left(-\frac{\mathcal{H}(\sigma)}{k_B T}\right)$$

partition sum $Z = \sum_\sigma \exp(-\mathcal{H}(\sigma)/(k_B T))$

$p(\sigma) =$ probability to be in state σ

- Detailed Balance (strong condition for equilibrium)

$$p(\sigma)W(\sigma \to \tau) = p(\tau)W(\tau \to \sigma)$$

$W(\sigma \to \tau) =$ transition probability from the state σ to the state τ

$$\frac{W(\sigma \to \tau)}{W(\tau \to \sigma)} = \frac{p(\tau)}{p(\sigma)} = \exp\left(-\frac{\Delta\mathcal{H}}{k_B T}\right)$$

Some arbitrariness in the explicit choice of W remains.

$\longrightarrow$ Metropolis Criterion

$$W(\sigma \to \tau) = \min\left\{1, \exp\left(-\frac{\Delta\mathcal{H}}{k_B T}\right)\right\} = \begin{cases} \exp\left(-\frac{\Delta\mathcal{H}}{k_B T}\right) & \text{if } \Delta\mathcal{H} \geq 0 \\ 1 & \text{otherwise} \end{cases}$$

or Heatbath Criterion

$$W(\sigma \to \tau) = \frac{p(\tau)}{p(\sigma) + p(\tau)} = \frac{1}{1 + \exp\left(\frac{\Delta\mathcal{H}}{k_B T}\right)}$$

Algorithms related to Simulated Annealing

Threshold Accepting

$$W(\sigma \to \tau) = \begin{cases} 1 & \text{if } \Delta\mathcal{H} \leq Th \\ 0 & \text{otherwise} \end{cases}$$

Great Deluge Algorithm

$$W(\sigma \to \tau) = \begin{cases} 1 & \text{if } \mathcal{H}(\tau) \leq \mathcal{T} \\ 0 & \text{otherwise} \end{cases}$$

Penna Criterion

$$W(\sigma \to \tau) = \min \left\{ 1, \left(1 - (1-q)\frac{\Delta\mathcal{H}}{kT} \right)^{\frac{1}{1-q}} \right\}$$

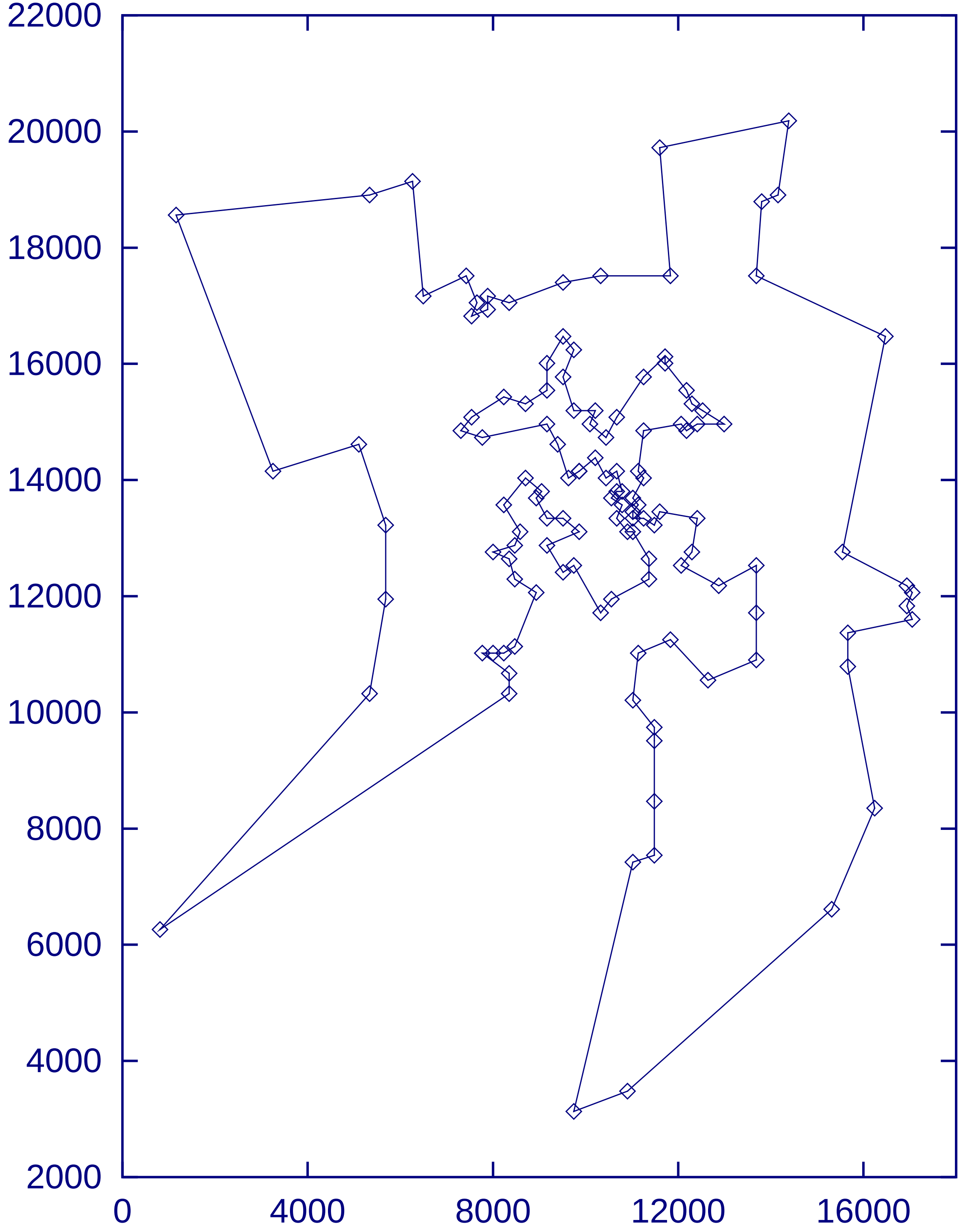
Working Horse

The Standard Problem of Optimization

The Traveling Salesman Problem (TSP)

Benchmark libraries

Benchmark instances like BEER127, PCB442, and ATT532



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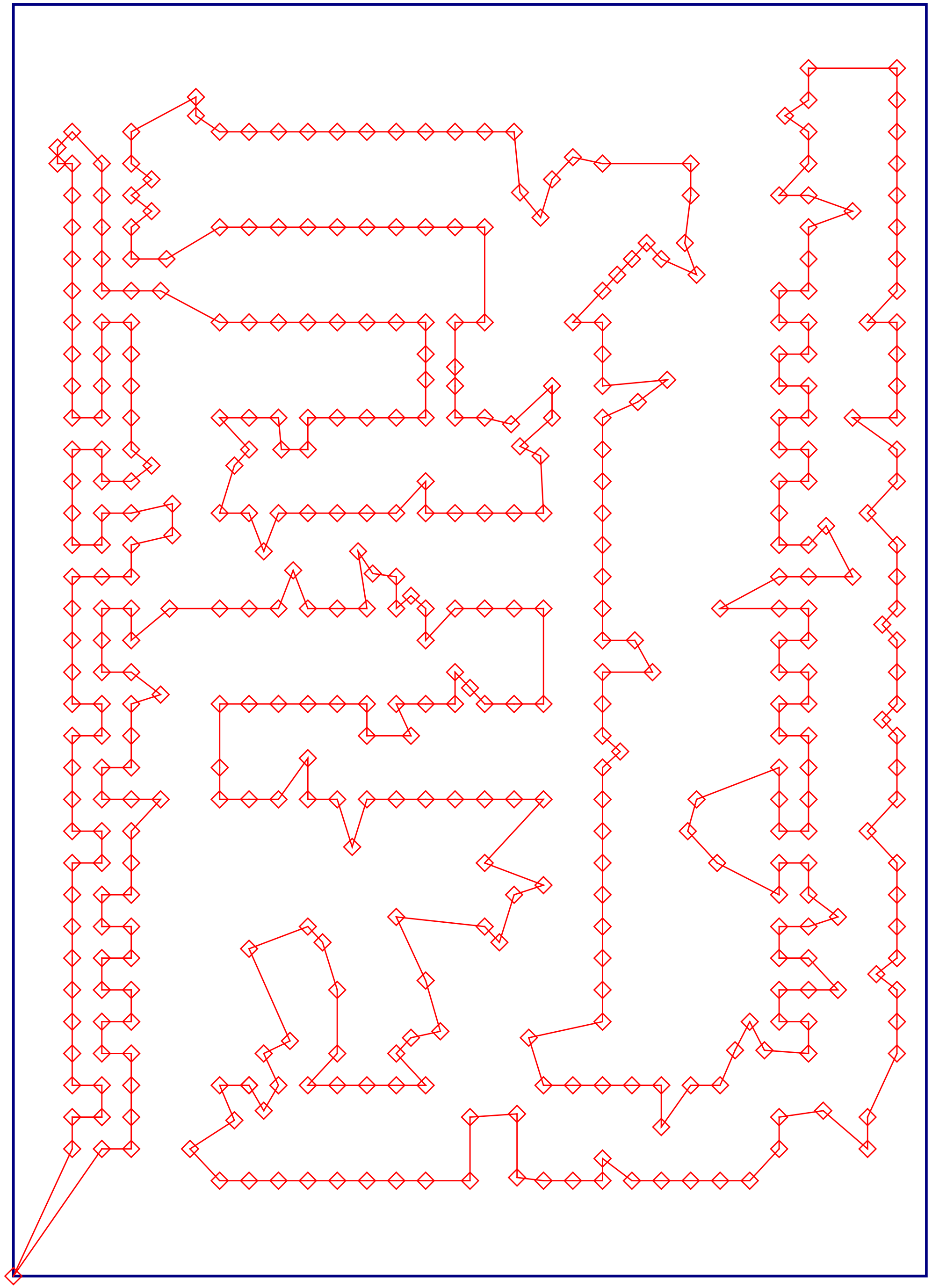
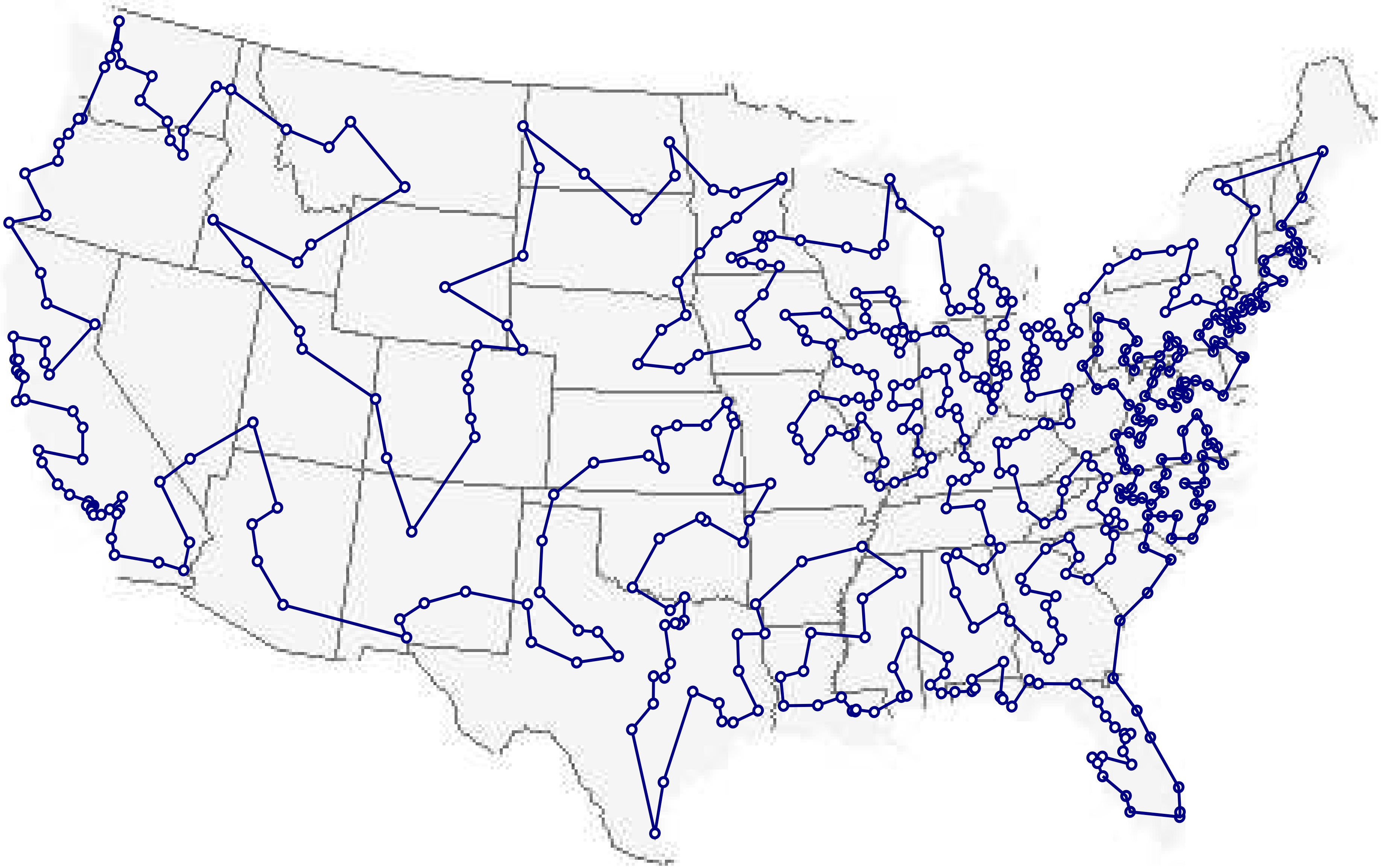
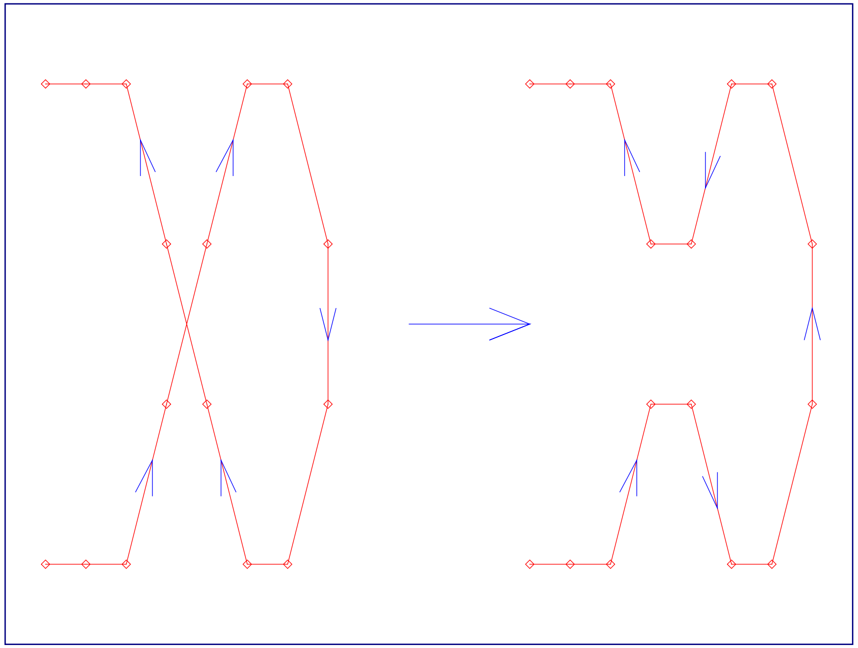


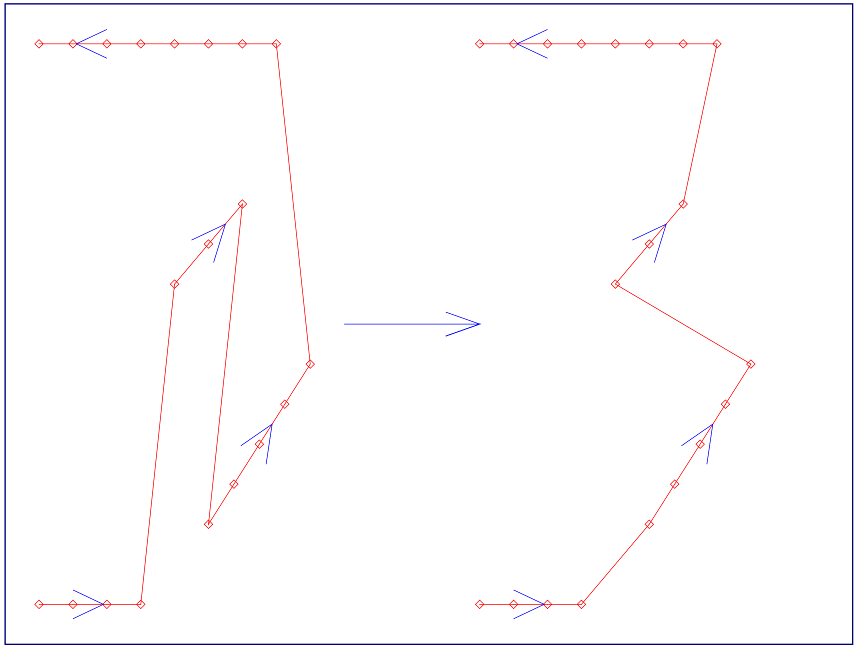


Moves for the TSP

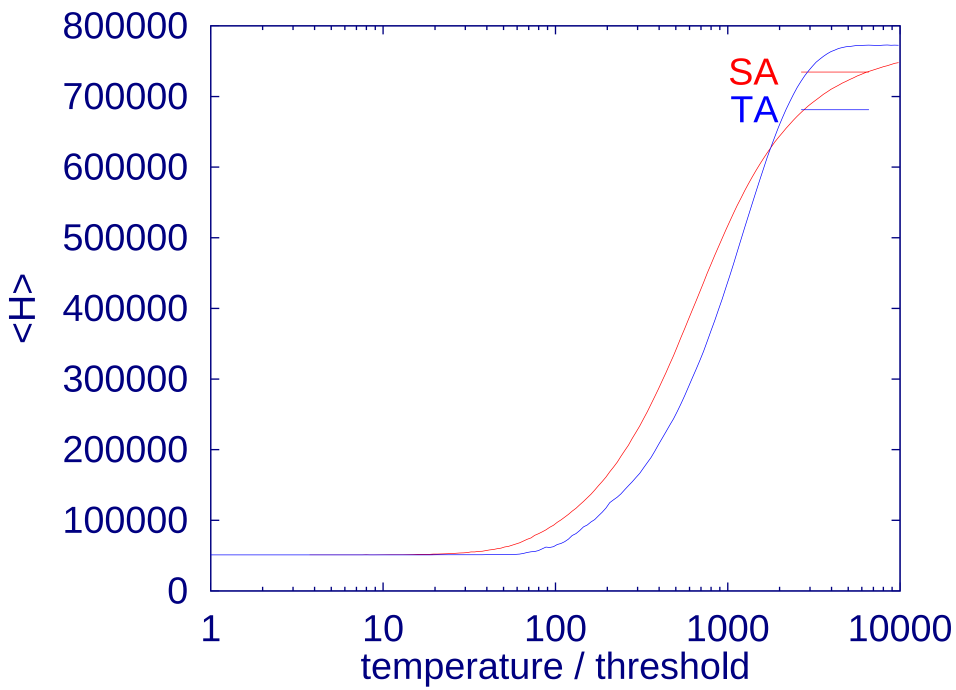
Lin-2-Opt

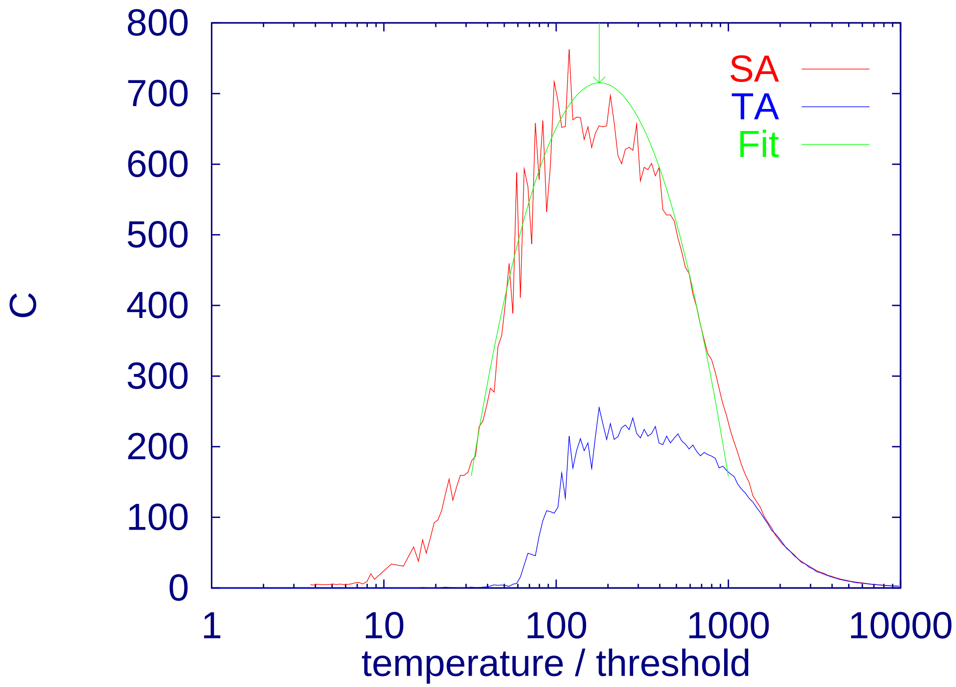


Lin-3-Opt



Results





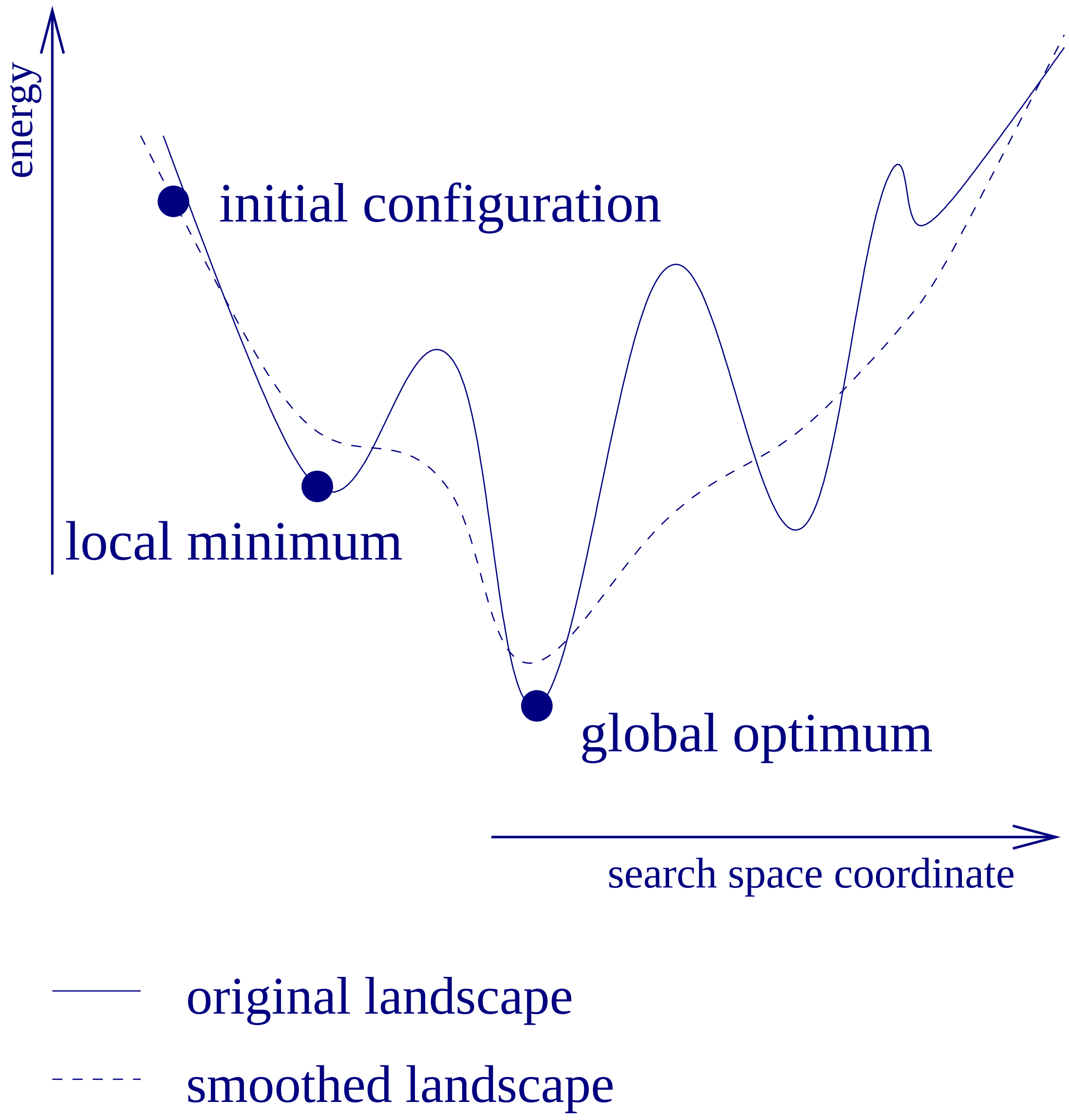
$$\langle \mathcal{H} \rangle = \frac{1}{Z} \sum_{\sigma} \mathcal{H}(\sigma) \exp\left(-\frac{\mathcal{H}(\sigma)}{k_B T} \right)$$

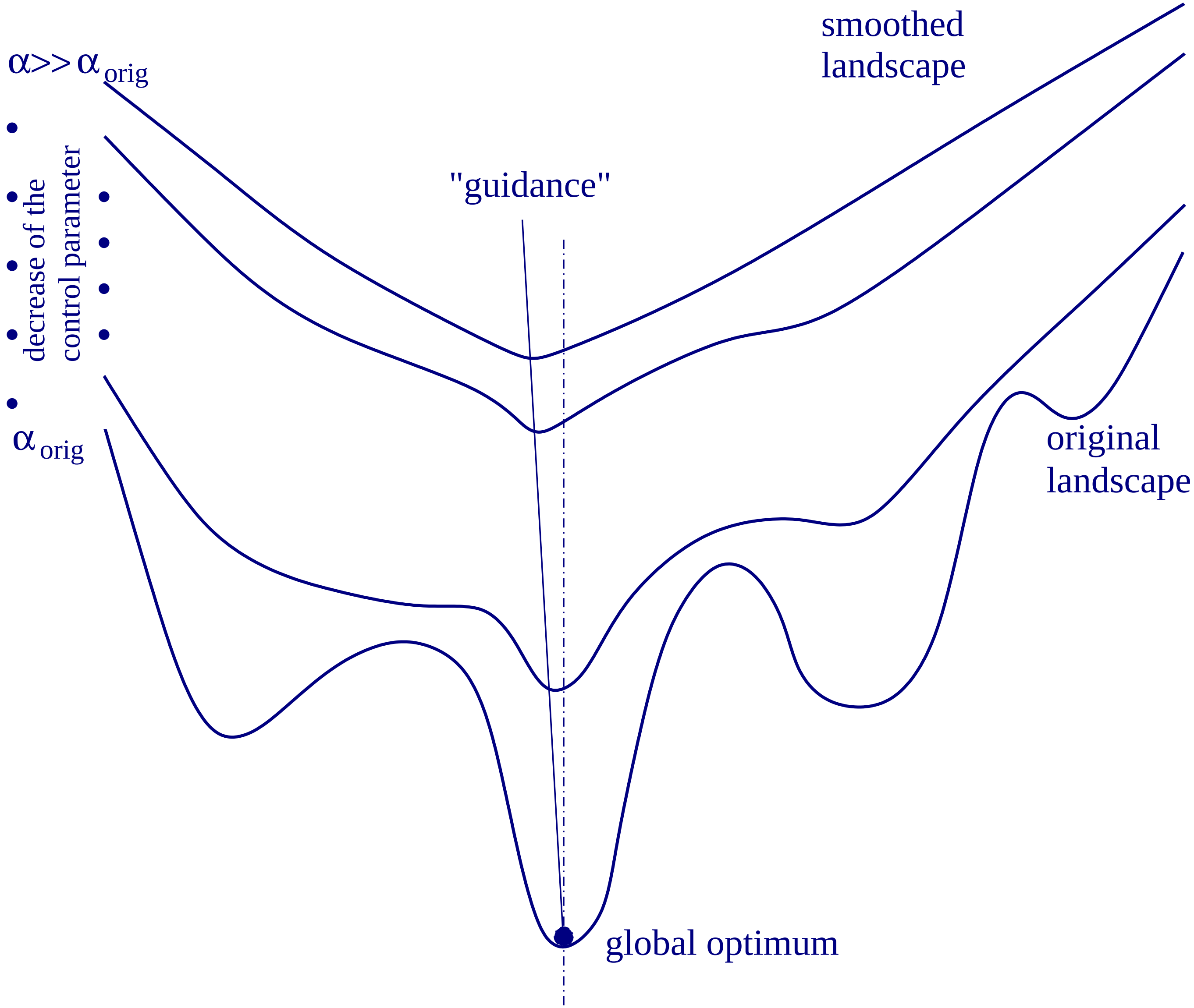
$$C = \frac{\partial \langle \mathcal{H} \rangle}{\partial T} = \frac{\mathrm{Var}(\mathcal{H})}{k_B T^2}$$

Methods to Increase the Efficiency

- Choice of the Control Parameter
- Choice of the Cooling Schedule
- Choice of the Moves

Search Space Smoothing





α>>α orig
decrease of the
control parameter
α orig
"guidance"
smoothed
landscape
original
landscape
global optimum

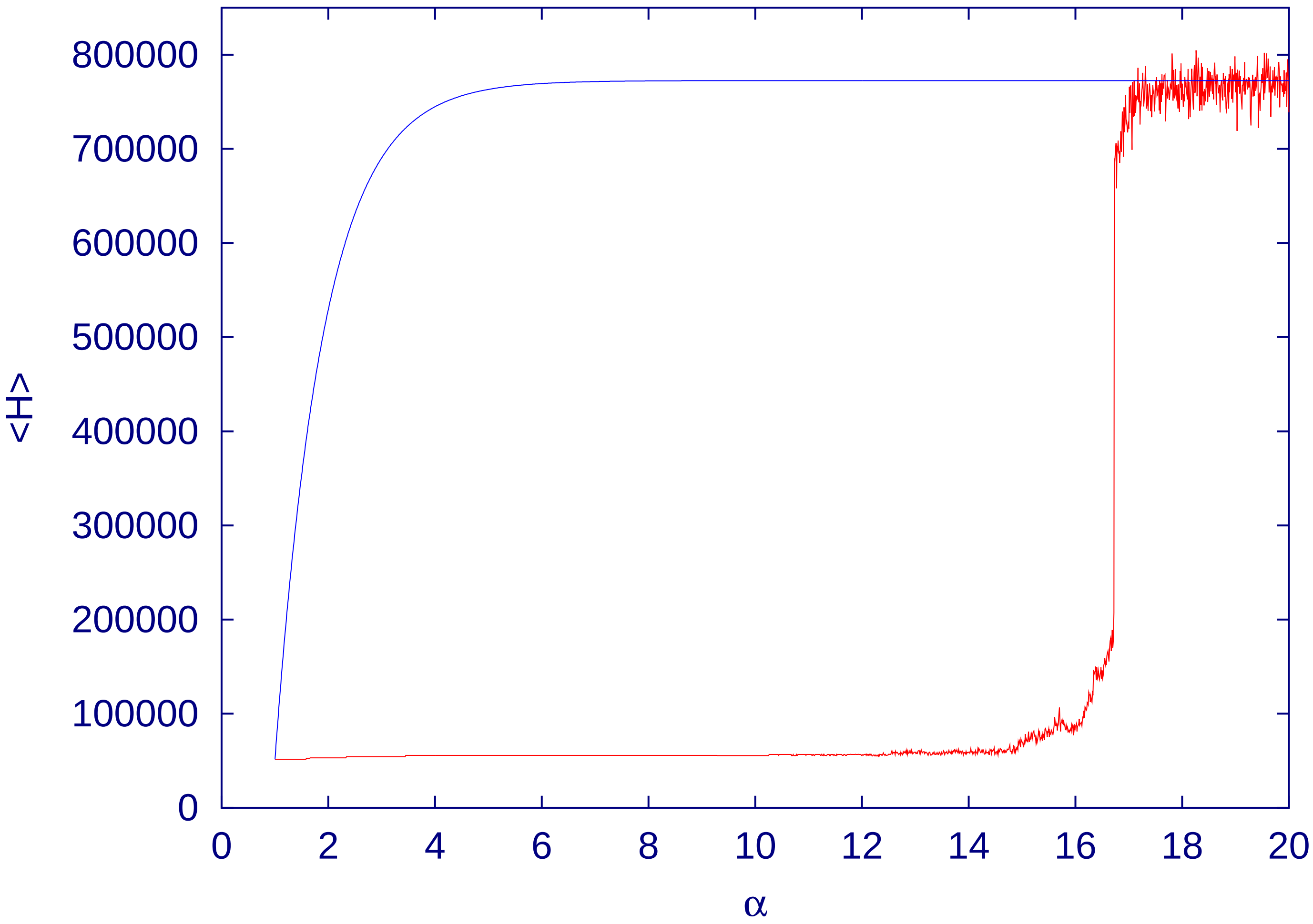
Search Space Smoothing

normalized distances $d(i,j) = D(i,j)/D_{\mathrm{max}}$

mean distance

$$\bar{d} = \frac{1}{N(N-1)} \sum_{i,j=1}^{N} d(i,j)$$

$$d_\alpha(i,j) = \begin{cases} \bar{d} + \left(d(i,j) - \bar{d}\right)^\alpha & \text{if } d(i,j) \geq \bar{d} \\ \bar{d} - \left(\bar{d} - d(i,j)\right)^\alpha & \text{otherwise} \end{cases}$$



red curve according to the original distances

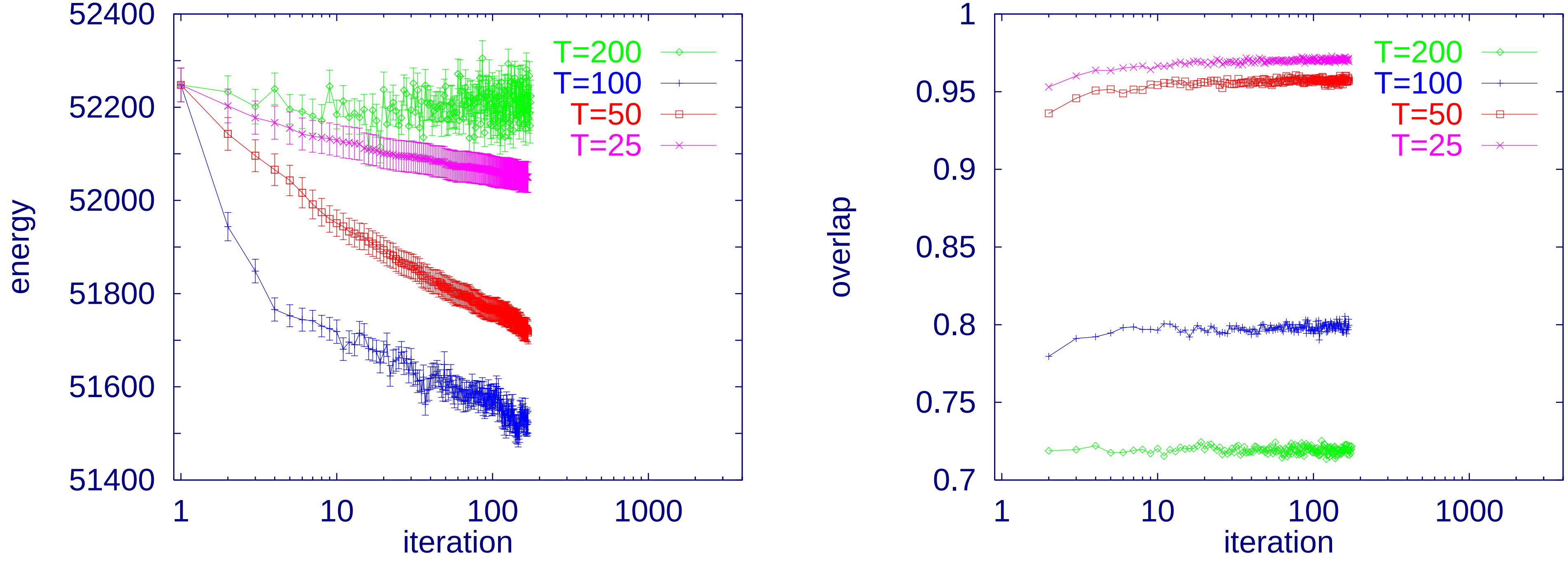
blue curve according to the unsmoothed distances

(unnormalized)

Bouncing

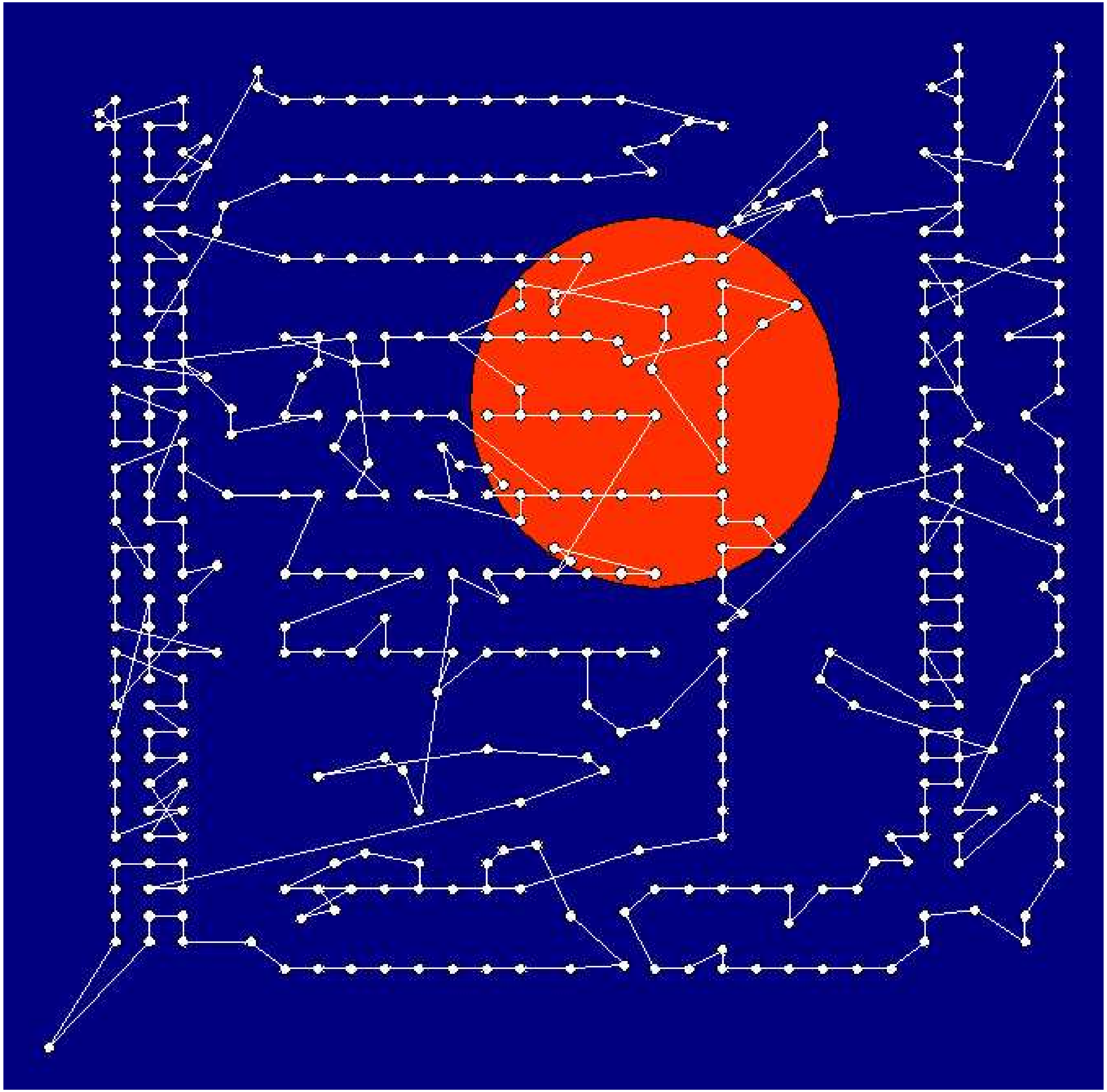
classic ansatz: monotonous cooling

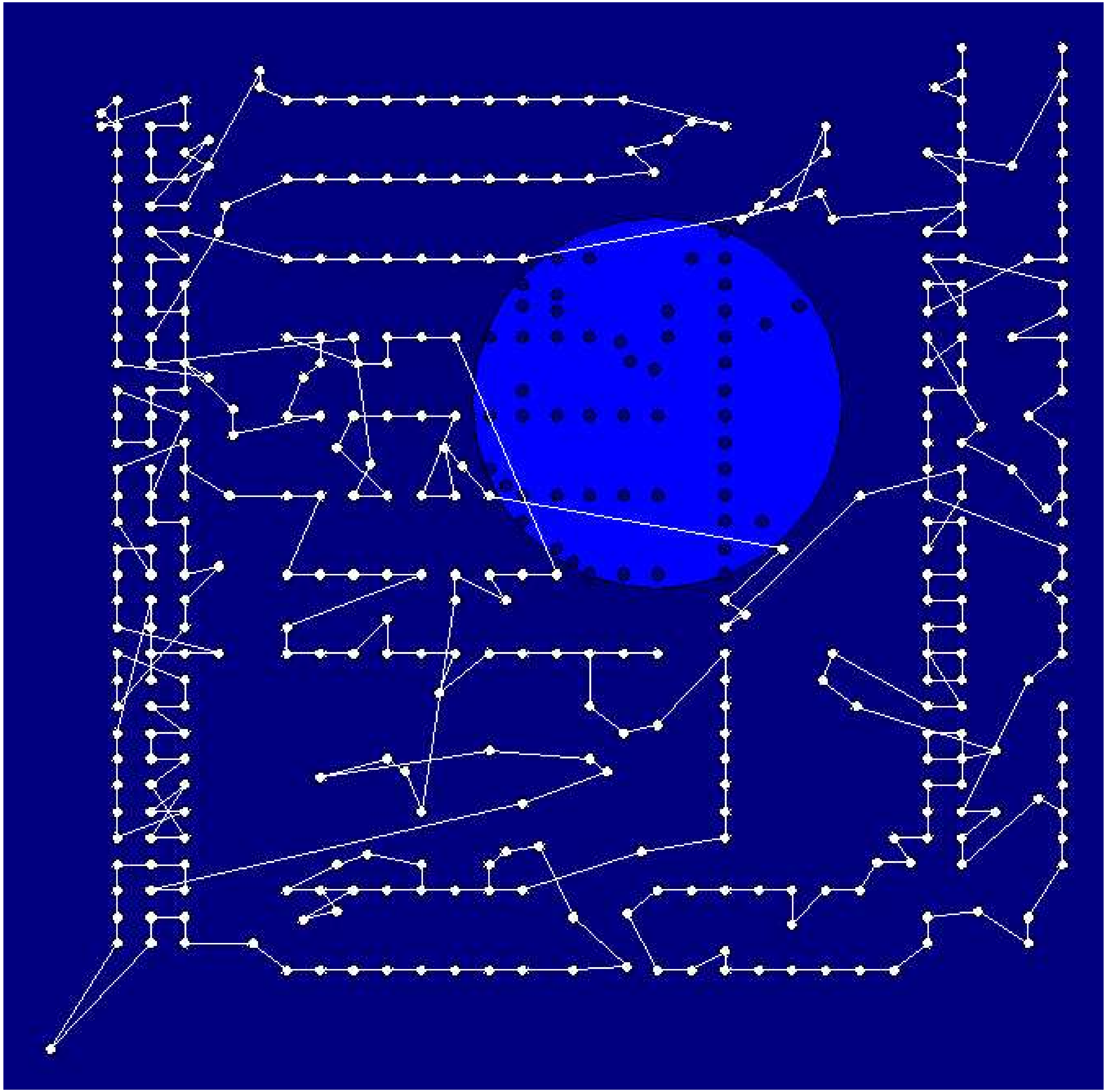
new ansatz: iterated cooling and reheating of the system

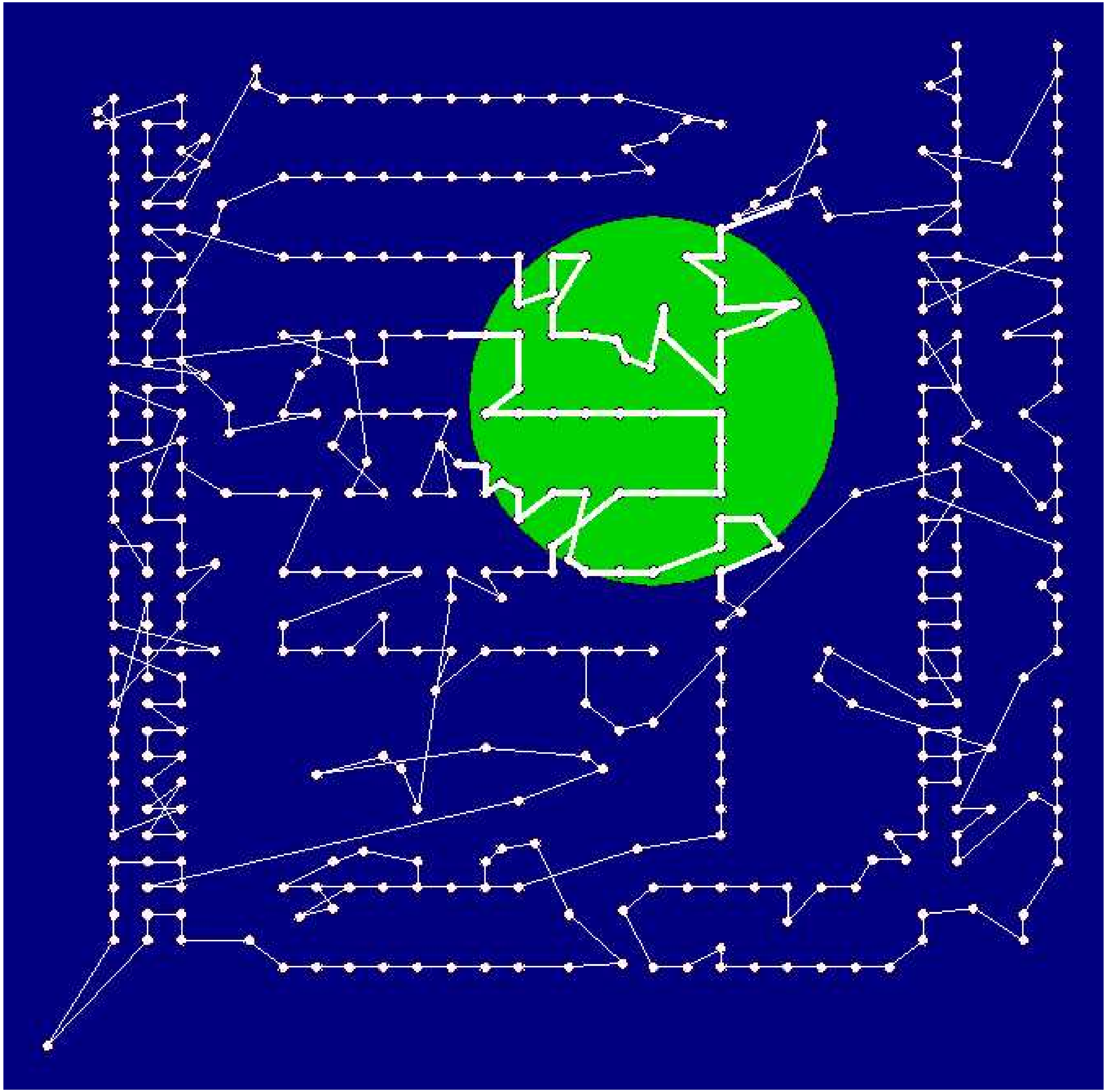


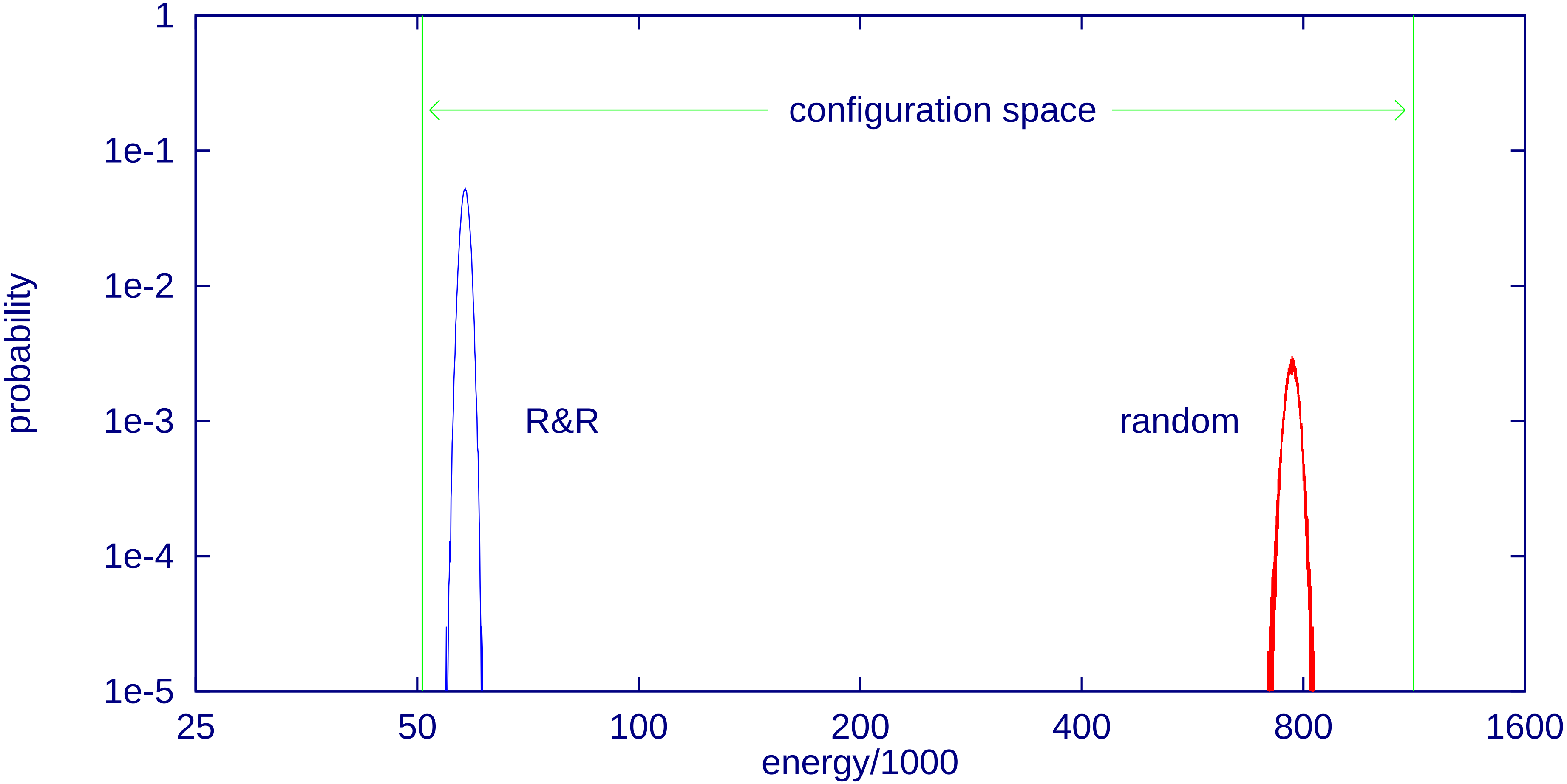
Ruin & Recreate

classic ansatz:	small local change
new ansatz:	destruction and intelligent recreation of a larger system part

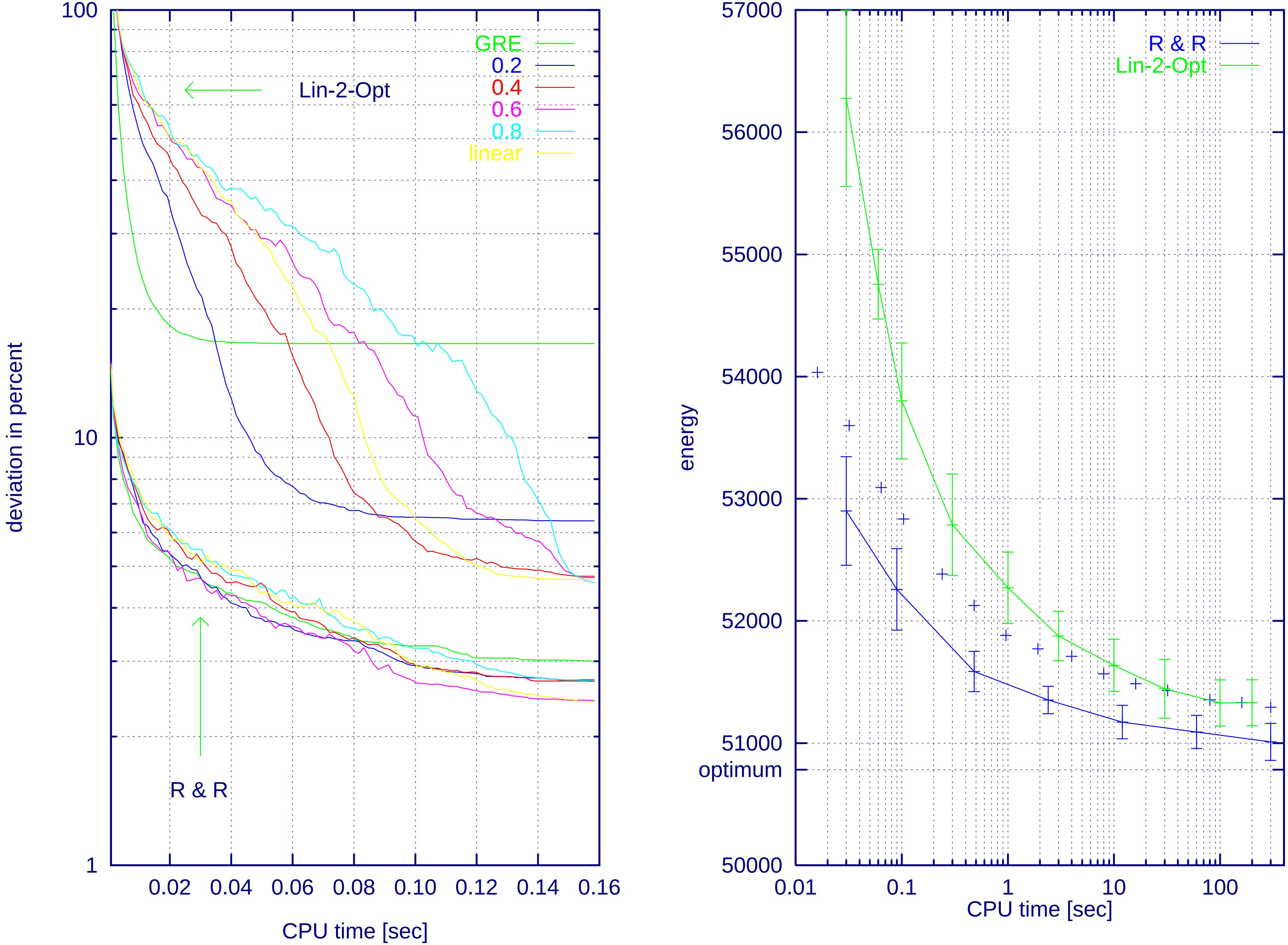








configuration space
R&R
random
probability
energy/1000
1
1e-1
1e-2
1e-3
1e-4
1e-5
25
50
100
200
400
800
1600

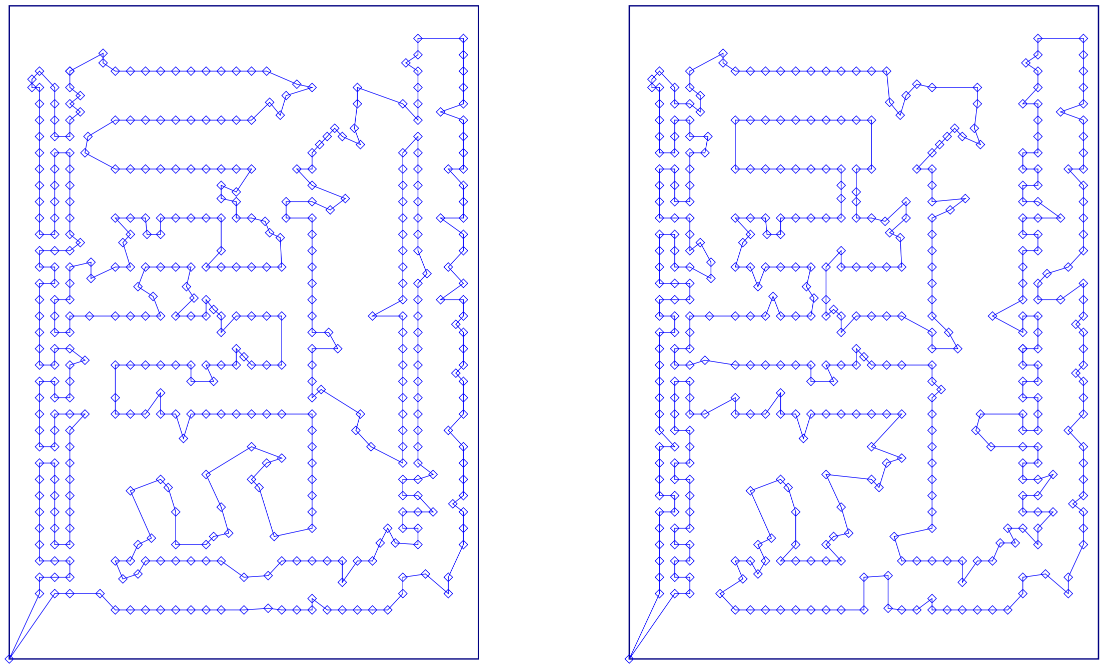


100
10
1
deviation in percent
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
CPU time [sec]
GRE
0.2
0.4
0.6
0.8
linear
Lin-2-Opt
R & R
57000
56000
55000
54000
53000
52000
51000
optimum
50000
energy
0.01
0.1
1
10
100
CPU time [sec]
R & R
Lin-2-Opt

Approaches for Parallelization

- Splitting of the Problem into Subproblems
- Information Exchange during the Optimization Run
- Information Exchange after the Optimization Run

Searching for Backbones

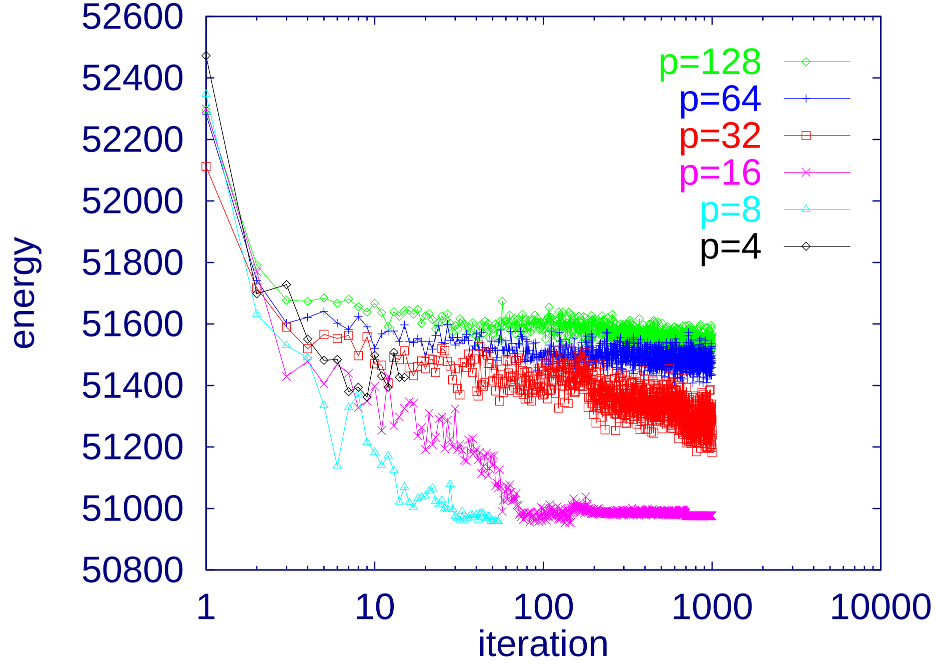


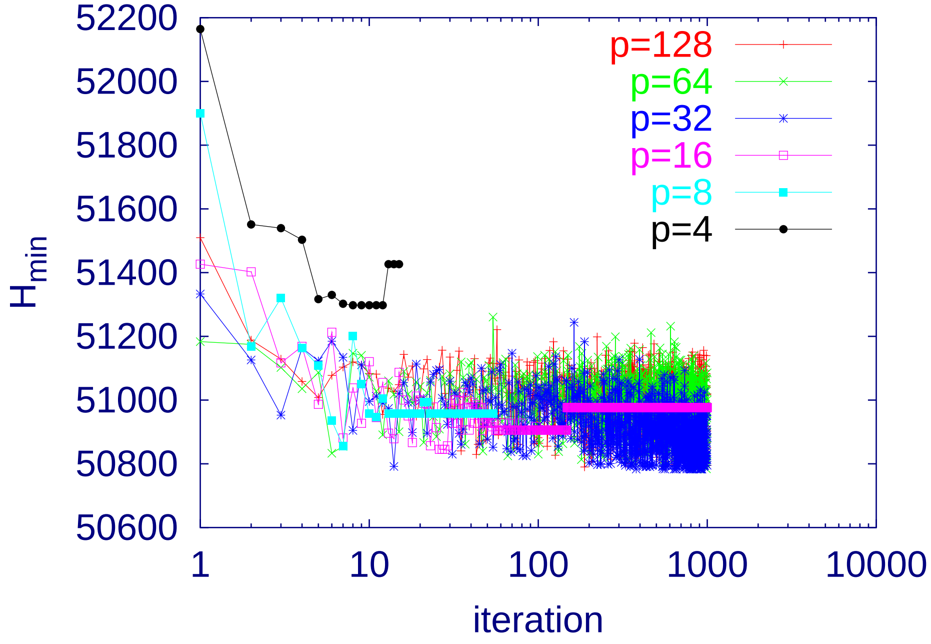
Finding common structures in different solutions and eliminating them in order to save calculation time and achieve better solutions

Outline of the Searching for Backbones Algorithm

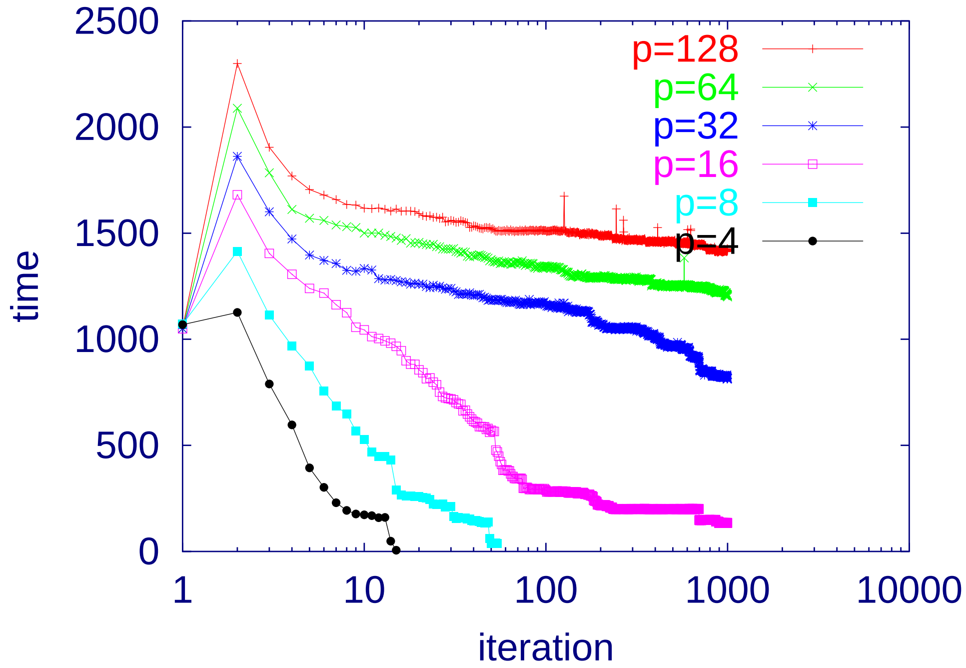
1. Perform several independent optimization runs.
2. Compare the achieved solutions for common parts.
3. Assume these common parts to be optimally solved and to be part of the optimum solution.
4. Perform again several independent optimization runs, but now keeping the found backbones constant during the optimization run.
5. If the solutions differ, return to step 2.

Quality of the Results

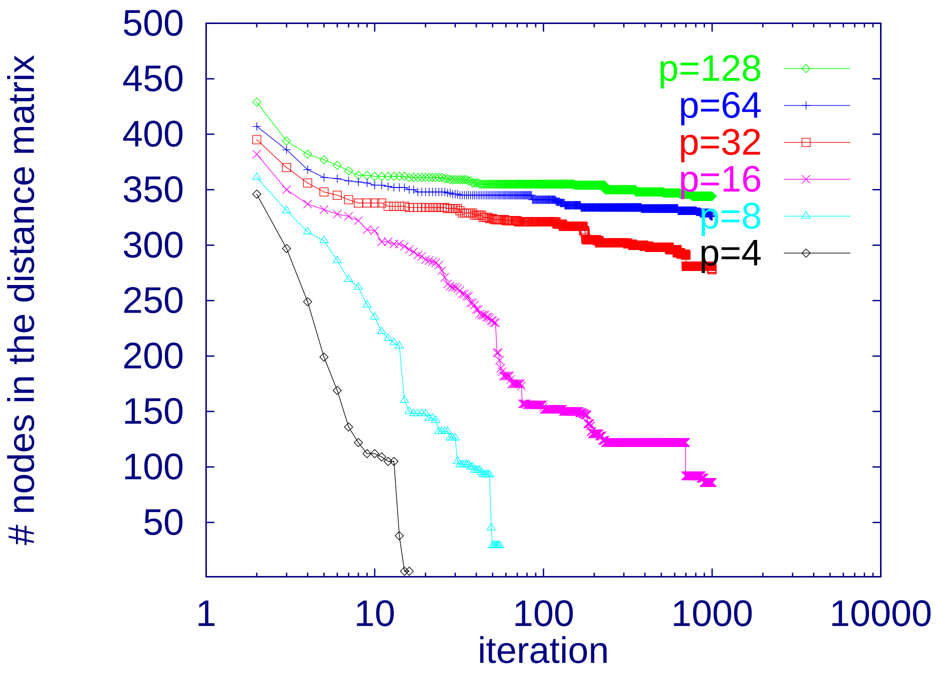


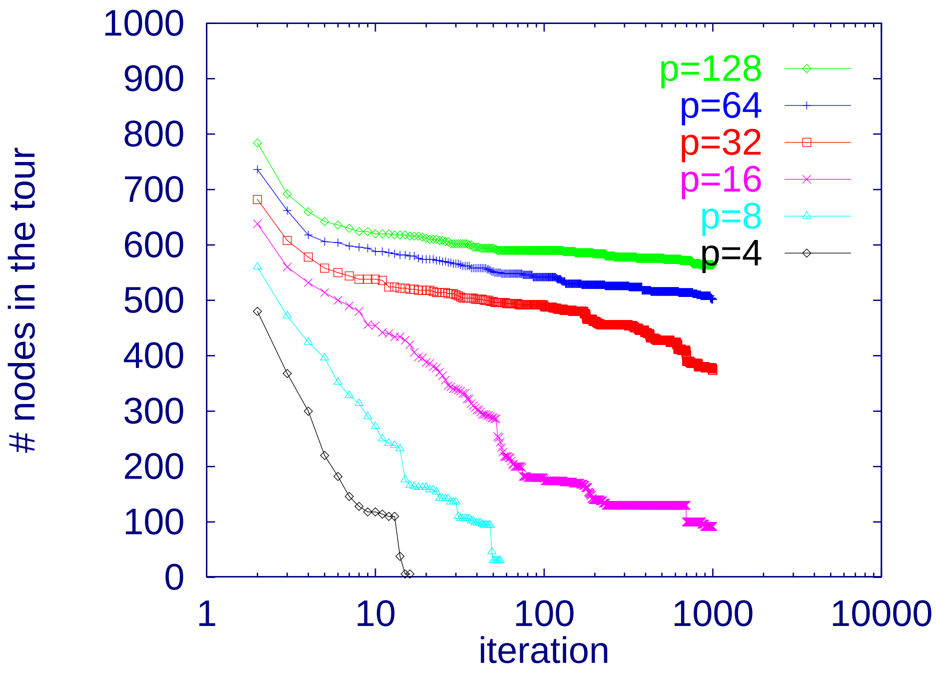


Calculation Time



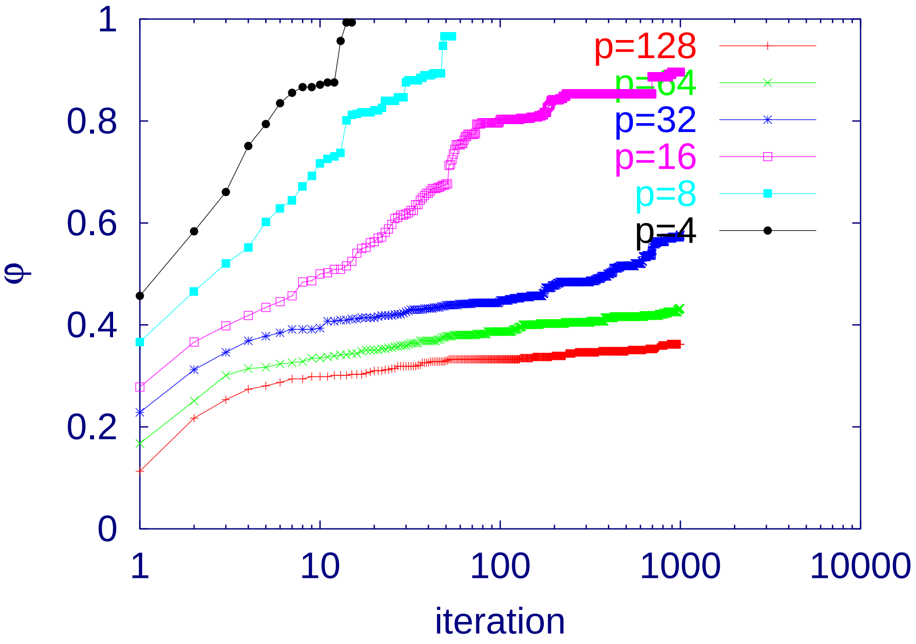
Convergence behavior of the algorithm

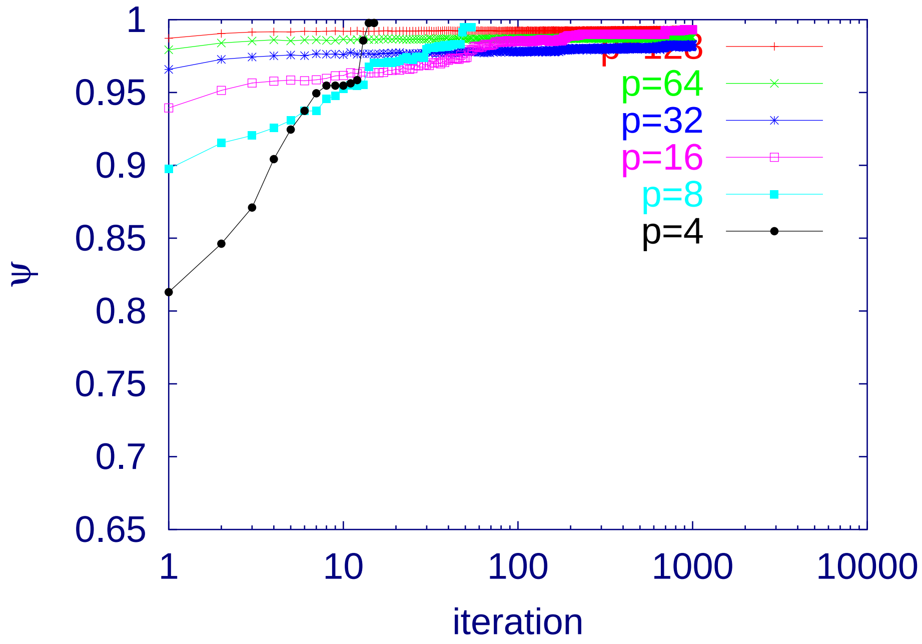




Order Parameters

$$\varphi(\eta) = \frac{\sum_{i,j} \delta_{\eta(i,j),p}}{2N} \qquad \psi(\eta) = 1 - \frac{-2N + \sum_{i,j}(1 - \delta_{\eta(i,j),0})}{2N(p-1)}$$



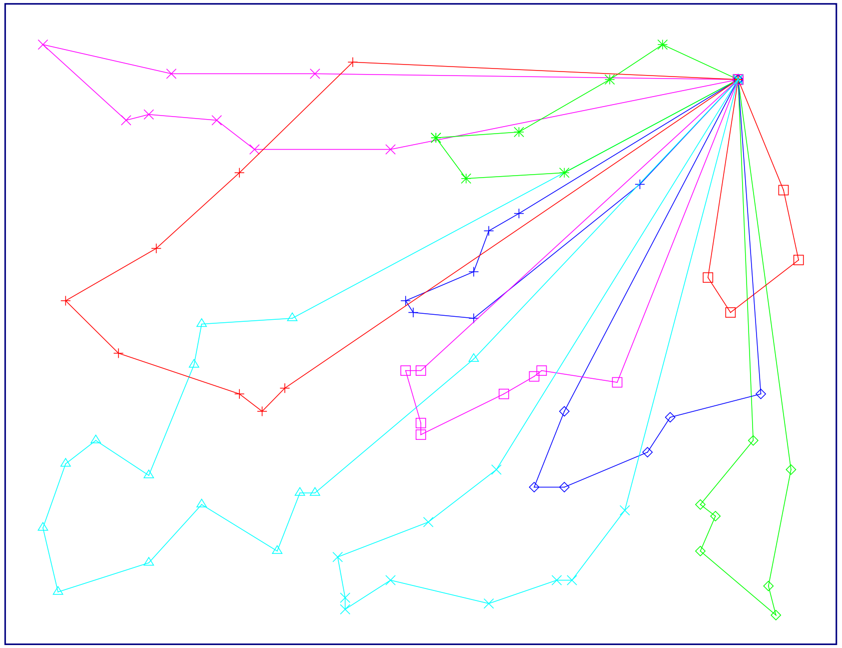


Applications to Other Problems

Vehicle Routing Problems

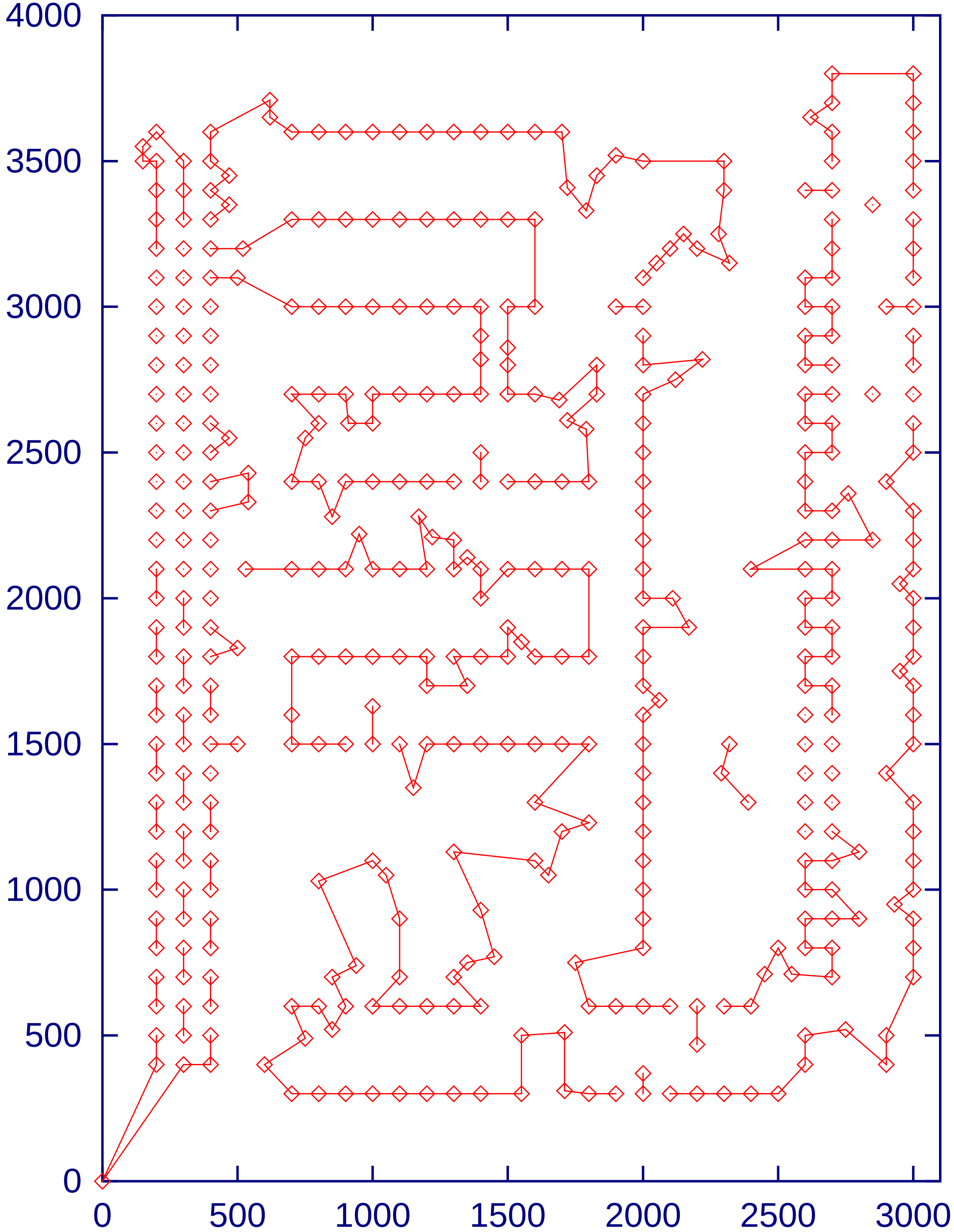
TSP $\longrightarrow$ MTSP $\longrightarrow$ VRP

A-n80-k10



Add a penalty function with a Lagrange multiplier λ to fulfill the capacity constraint:

$$
\begin{aligned}
\mathcal{H}(\sigma) \;=\; & \sum_{l=1}^{L} \quad \sum_{i=1}^{N_l-1} D(\sigma(i,l),\sigma(i+1,l)) \\
& + \;\; \lambda \sum_{l=1}^{L} \left(\sum_{i=2}^{N_l-1} m(\sigma(i,l)) - \kappa + \gamma \right) \\
& \qquad \ominus \left(\sum_{i=2}^{N_l-1} m(\sigma(i,l)) - \kappa \right)
\end{aligned}
$$

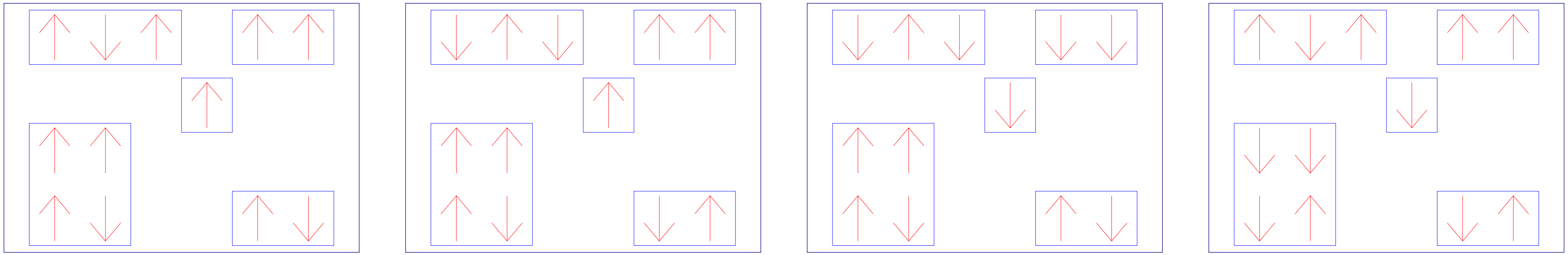

4000
3500
3000
2500
2000
1500
1000
500
0
0
500
1000
1500
2000
2500
3000

Spin Glasses

SK model

$$\mathcal{H} = -\sum_{i,j} J_{ij} S_i S_j$$

with $S_i = \pm 1$ and $P(J_{ij}) \propto \exp(-J_{ij}^2/2)$



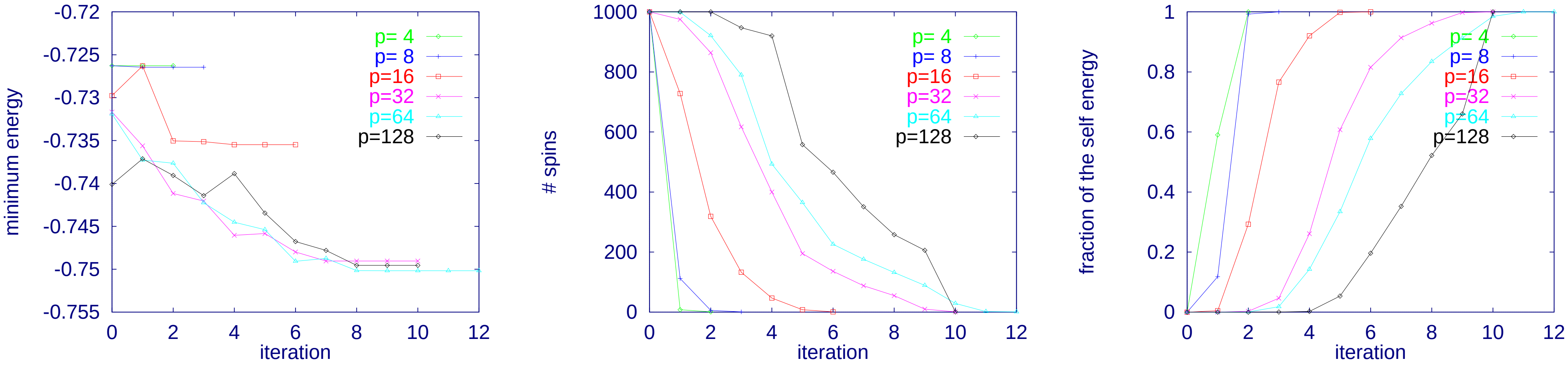
Searching for Backbones

$$\eta(i,j) = \left| \sum_{\nu=1}^{p} S_i^\nu \cdot S_j^\nu \right|$$

Spins i and j can be put together to one backbone spin α if $\eta(i,j) = p$.

Hamiltonian for backbone spins:

$$\mathcal{H} = -\sum_{\alpha,\beta} J_{\alpha\beta} S_\alpha S_\beta \quad \text{with} \quad J_{\alpha\beta} S_\alpha S_\beta = \sum_{\substack{i\in\alpha \\ j\in\beta}} J_{ij} S_i^\xi S_j^\xi$$



References

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