Simulated Annealing

A Basic Introduction

Lecture 10

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Outline

- Heuristics
- Background in Statistical Mechanics
  - Atom Configuration Problem
  - Metropolis Algorithm
- Simulated Annealing Algorithm
- Sample Problems and Applications
- Summary

Learning Objectives

- Review background in Statistical Mechanics: configuration, ensemble, entropy, heat capacity

- Understand the basic assumptions and steps in Simulated Annealing (SA)

- Be able to transform design problems into a combinatorial optimization problem suitable to SA

- Understand strengths and weaknesses of SA

Heuristics

What is a Heuristic?

- A Heuristic is simply a rule of thumb that hopefully will find a good answer.

- Why use a Heuristic?

    - Heuristics are typically used to solve complex (large, nonlinear, non-convex (i.e. contain local minima)) multivariate combinatorial optimization problems that are difficult to solve to optimality.

- Unlike gradient-based methods in a convex design space, heuristics are NOT guaranteed to find the true global optimal solution in a single objective problem, but should find many good solutions (the mathematician's answer vs. the engineer's answer)

- Heuristics are good at dealing with local optima without getting stuck in them while searching for the global optimum.

Types of Heuristics

- Heuristics Often Incorporate Randomization

- **Two Special Cases of Heuristics**
  - Construction Methods
    - Must first find a feasible solution and then improve it.
  - Improvement Methods
    - Start with a feasible solution and just try to improve it.

- **3 Most Common Heuristic Techniques**
  - Simulated Annealing
  - Genetic Algorithms
  - Tabu Search
  - New Methods: Particle Swarm Optimization, etc…

Origin of Simulated Annealing (SA)

- **Definition**: A heuristic technique that mathematically mirrors the cooling of a set of atoms to a state of minimum energy.

- **Origin:** Applying the field of Statistical Mechanics to the field of Combinatorial Optimization (1983)

- Draws an **analogy** between the cooling of a material (search for minimum energy state) and the solving of an optimization problem.

- **Original Paper** Introducing the Concept
  - Kirkpatrick, S., Gelatt, C.D., and Vecchi, M.P., "Optimization by Simulated Annealing," *Science*, Volume 220, Number 4598, 13 May 1983, pp. 671-680.
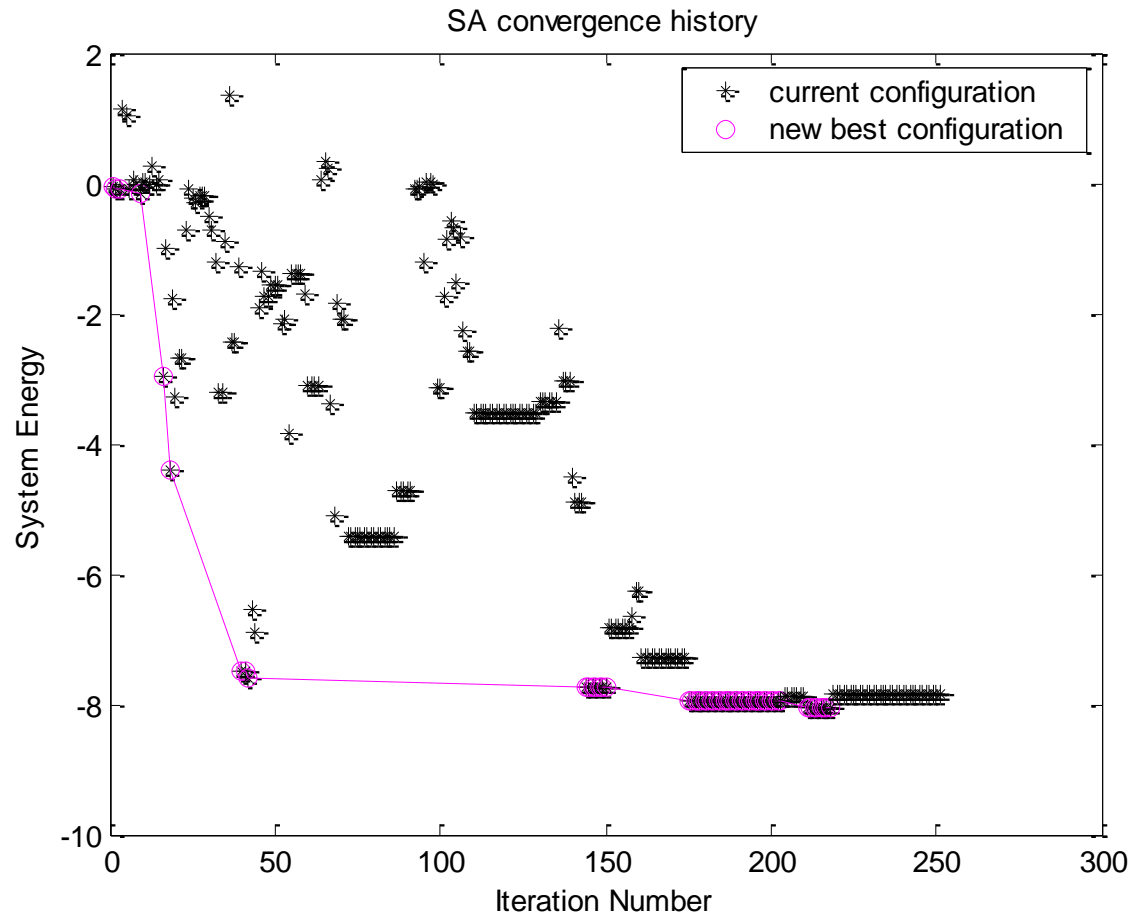
MATLAB® "peaks" function

- Difficult due to plateau at z=0, local maxima
- SAdemo1
- x_o=[-2,-2]
- Optimum at
- x*=[0.012, 1.524]
- z*=8.0484

Peaks

Maximum

Start Point
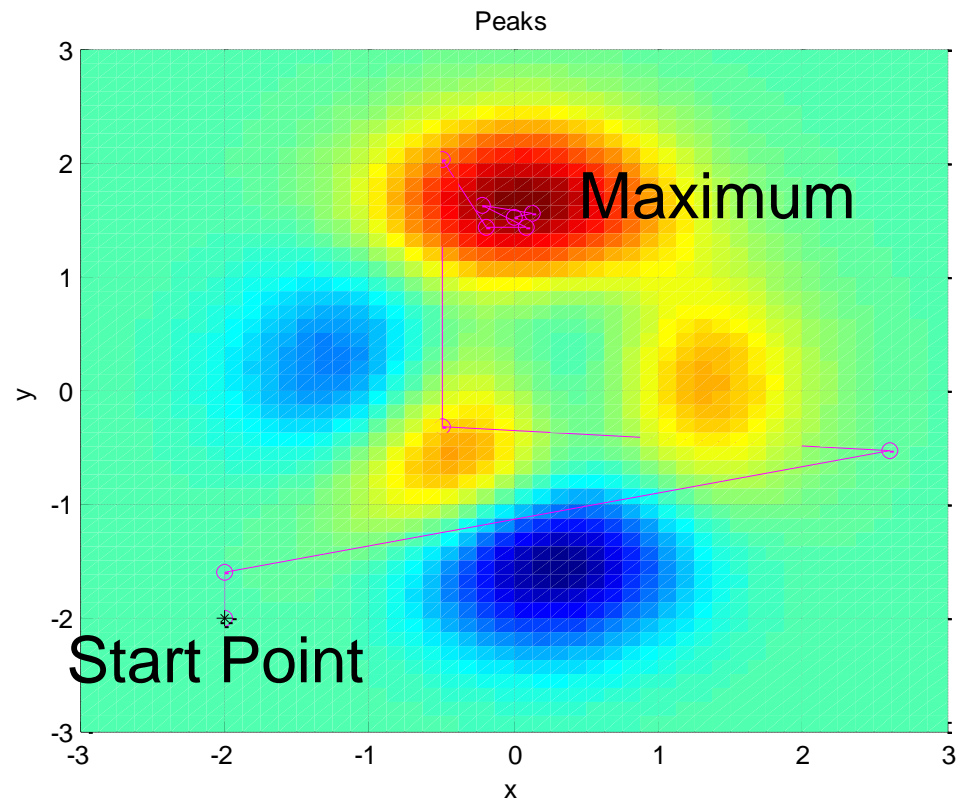
"peaks" convergence

- Initially ~ nearly random search
- Later ~ gradient search

SA convergence history

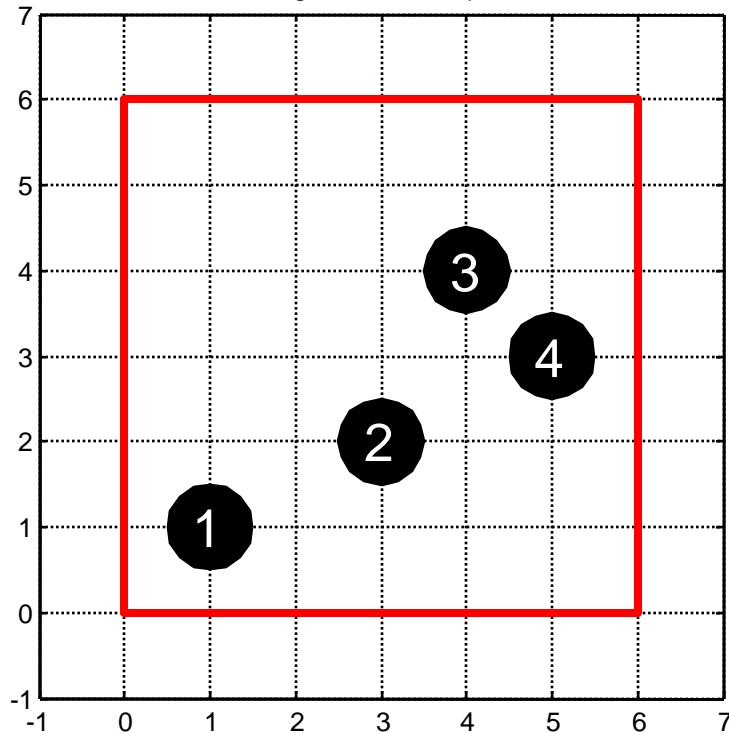# Statistical Mechanics

The Analogy

- **Statistical Mechanics:** The behavior of systems with many degrees of freedom in thermal equilibrium at a finite temperature.

- **Combinatorial Optimization:** Finding the minimum of a given function depending on many variables.

- **Analogy:** If a liquid material cools and anneals too quickly, then the material will solidify into a sub-optimal configuration. If the liquid material cools slowly, the crystals within the material will solidify optimally into a state of minimum energy (i.e. ground state).
    - This ground state corresponds to the minimum of the cost function in an optimization problem.
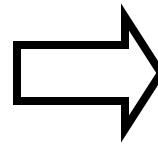
Sample Atom Configuration
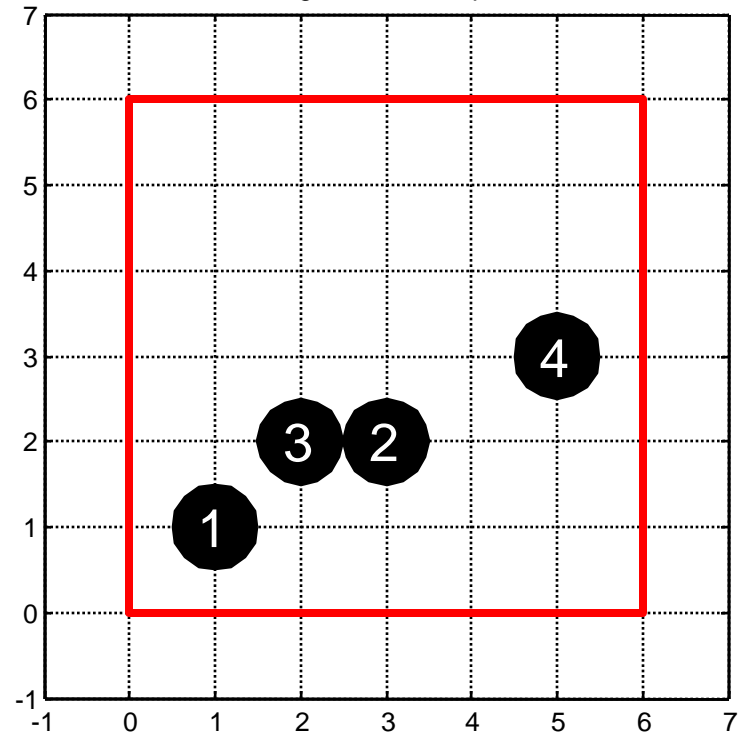
Original Configuration

Perturbed Configuration

Atom Configuration - Sample Problem

Atom Configuration - Sample Problem

E=133.67

E=109.04

Energy of original (configuration)

Perturbing = move a random atom to a new random (unoccupied) slot

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Configurations

- Mathematically describe a configuration
  - Specify coordinates of each "atom"

$$r_i \quad \text{with i=1,..,4} \quad r_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, r_2 = \begin{bmatrix} 3 \\ 2 \end{bmatrix}, r_3 = \begin{bmatrix} 4 \\ 4 \end{bmatrix}, r_4 = \begin{bmatrix} 5 \\ 3 \end{bmatrix}$$

  - Specify a slot for each atom

$$r_i \quad \text{with i=1,..,4} \quad R = \quad 1 \quad 12 \quad 19 \quad 23$$

Energy of a state

- Each state (configuration) has an energy level associated with it

$$H\left(q,\dot{q},t\right) = \sum_i \dot{q}_i p_i - L\left(q,\dot{q},t\right)$$ Hamiltonian

$$H = T + V = E_{tot}$$

↑ kinetic   ↑ potential

Energy

Energy of configuration
=
Objective function value of design

Energy sample problem

- Define energy function for "atom" sample problem

$$E_i = mgy_i + \sum_{j \neq i}^{N} \left[(x_i - x_j)^2 + (y_i - y_j)^2 \right]^{\frac{1}{2}}$$

$\underbrace{}$ potential energy

$\underbrace{\phantom{\sum_{j \neq i}^{N} (x_i - x_j)^2 + (y_i - y_j)^2}}$ kinetic energy

$$E(R) = \sum_{i=1}^{N} E_i(r_i)$$

Absolute and relative position of each atom contributes to Energy
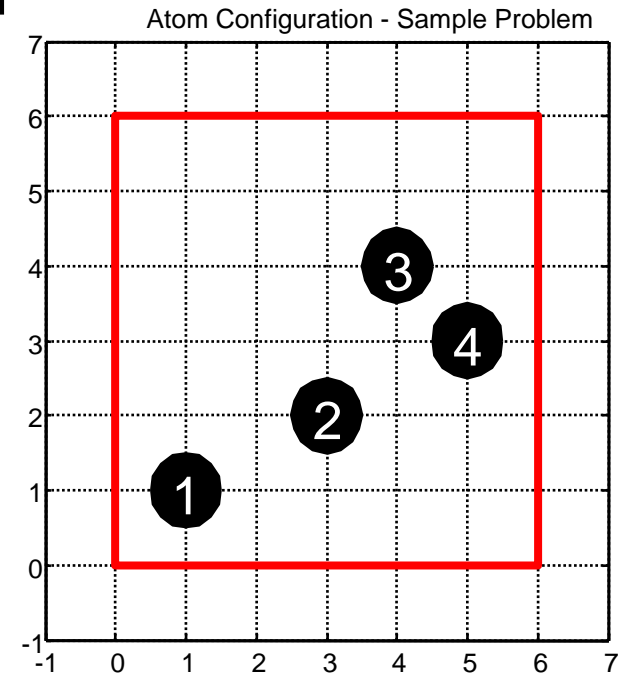
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Compute Energy of Config. A

- Energy of initial configuration

$$E_1 = 1 \cdot 10 \cdot 1 + \sqrt{5} + \sqrt{18} + \sqrt{20} = 20.95$$

$$E_2 = 1 \cdot 10 \cdot 2 + \sqrt{5} + \sqrt{5} + \sqrt{5} = 26.71$$

$$E_3 = 1 \cdot 10 \cdot 4 + \sqrt{18} + \sqrt{5} + \sqrt{2} = 47.89$$

$$E_4 = 1 \cdot 10 \cdot 3 + \sqrt{20} + \sqrt{5} + \sqrt{2} = 38.12$$

Atom Configuration - Sample Problem

Total Energy Configuration A: $E(\{r_A\}) = 133.67$

Boltzmann Probability

$$N_R = \frac{P!}{(P - N)!}$$

Number of configurations

P=# of slots=25
N=# of atoms =4

N_R=6,375,600

What is the likelihood that a particular configuration will exist in a large ensemble of configurations?

$$P\{r\} = \exp\left[\frac{-E(\{r\})}{k_B T}\right]$$

Boltzmann probability depends on energy and temperature
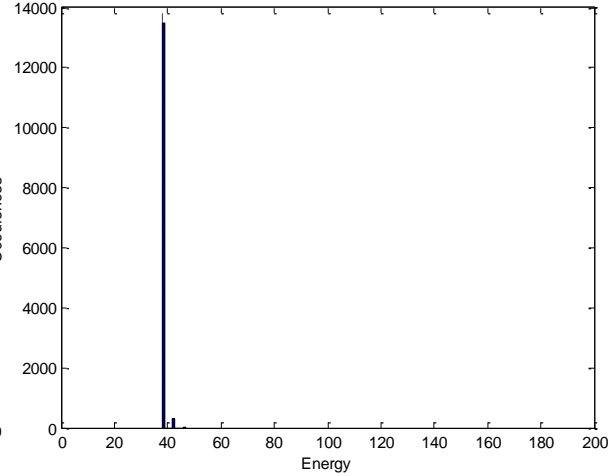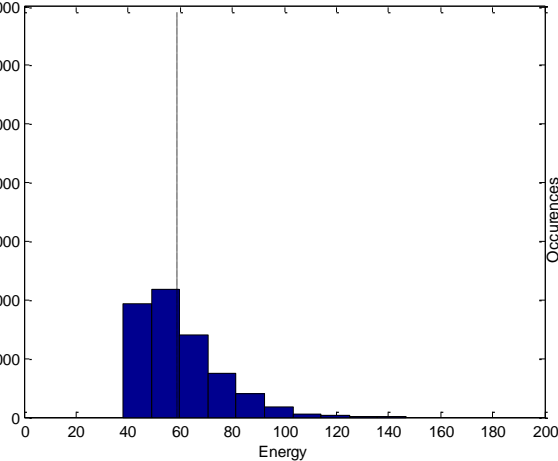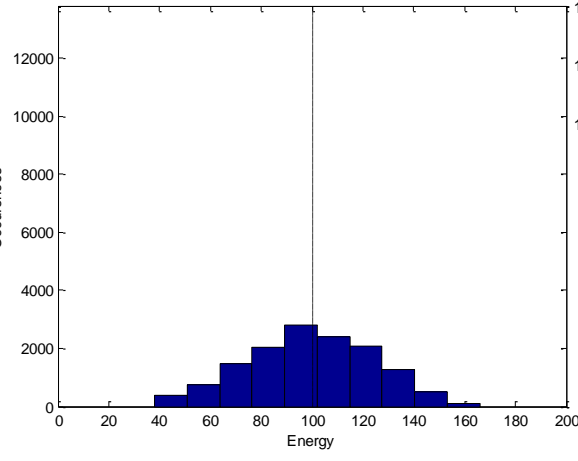
Boltzmann Collapse at low T

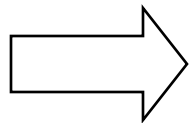T=100   T=10   T=1

T high ➡️ T low

Boltzmann Distribution collapses to the lowest energy state(s) in the limit of low temperature

➡️ Basis of search by Simulated Annealing

Partition Function Z

- Ensemble of configurations can be described statistically

- Partition function, Z, generates the ensemble average

$$Z = \mathrm{Tr}\exp\left(\frac{-E_i}{k_B T}\right) = \sum_{i=1}^{N_R}\exp\left(\frac{-E_i}{k_B T}\right)$$

Initially (at T>>0) equal to the number of possible configurations

Free Energy

$$E_{avg} = \overline{E}(T) = \sum_{i=1}^{N_R} E_i\left(T\right) \longleftarrow$$

Average Energy of all Configurations in an ensemble

$$F\left(T\right) = -k_B T \ln Z = \overline{E}(T) - TS$$

$$E_{avg} = \overline{E}(T) = \frac{\displaystyle\sum_{i=1}^{N_R} \exp\left(-\frac{E_i\left(T\right)}{k_B T}\right) E_i\left(T\right)}{Z} = \frac{-d \ln Z}{d\left(1/k_B T\right)}$$

Relates average Energy at T with Entropy S

Specific Heat and Entropy

- Specific Heat

$$C\left(T\right) = \frac{d\bar{E}(T)}{dT} = \frac{\left[\dfrac{1}{N_R}\displaystyle\sum_{i=1}^{N_R} E_i^2(T) - \overline{E\left(T\right)}^2\right]}{k_B T^2} = \frac{\overline{E^2(T)} - \overline{E\left(T\right)}^2}{k_B T^2}$$
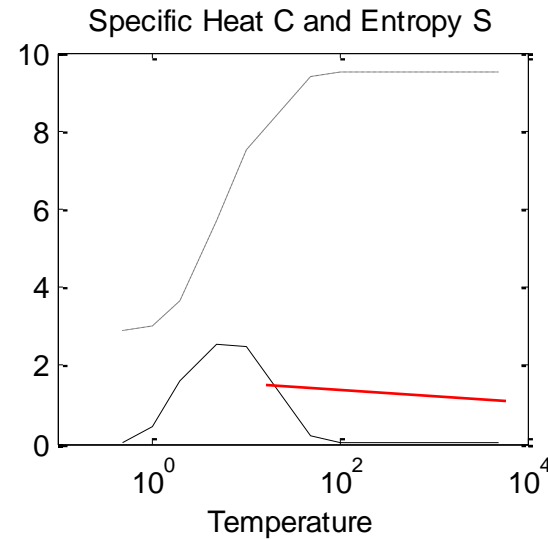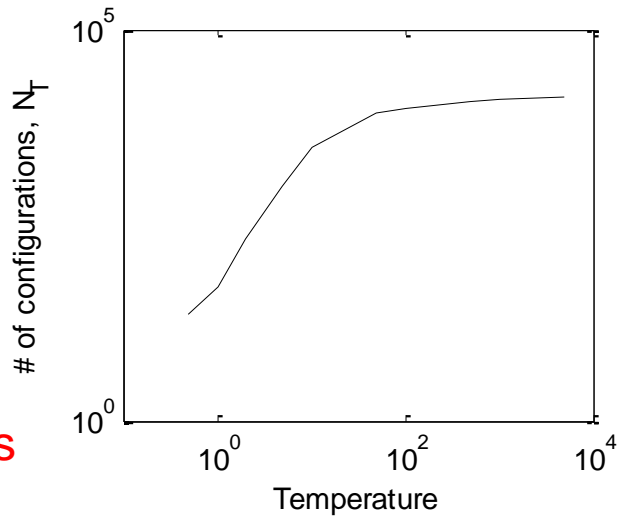
- Entropy

$$S(T) = S(T_1) - \int_T^{T_1} \frac{C(T)}{T}dT \qquad \frac{dS(T)}{dT} = \frac{C(T)}{T}$$

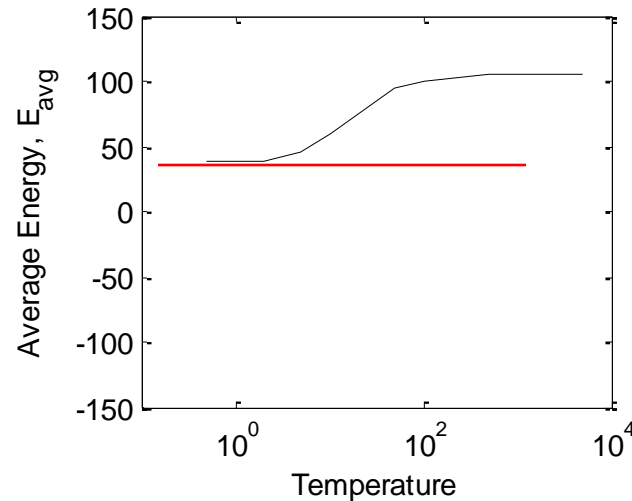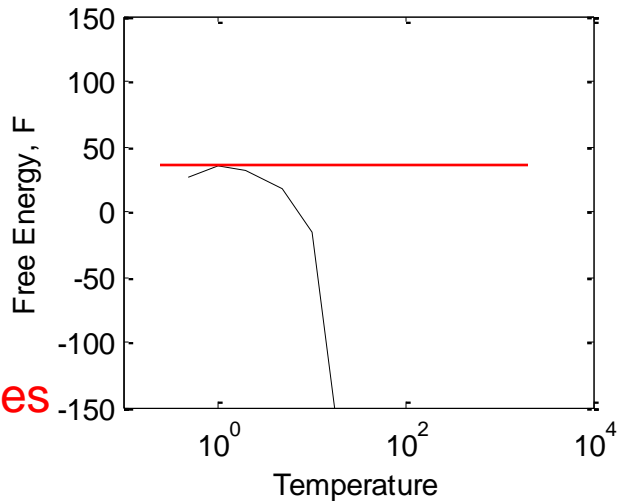Entropy is ~ equal to ln(# of unique configurations)

Low Temperature Statistics

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Minimum Energy Configurations

- Sample Atom Placement Problem

Uniqueness?

Atom Configuration - Sample Problem

E*=60

Strong gravity   g=10

Atom Configuration - Sample Problem

E*=14.26
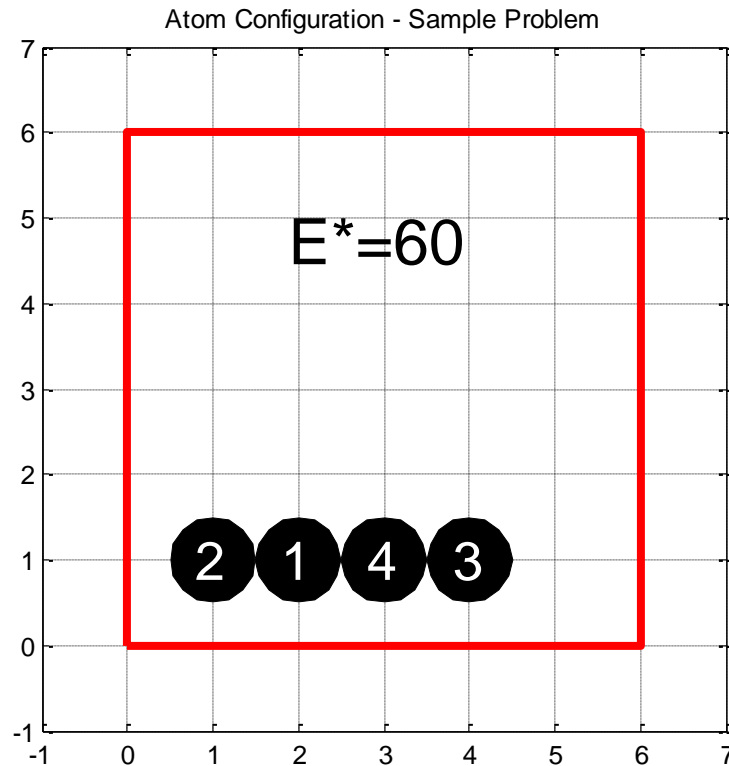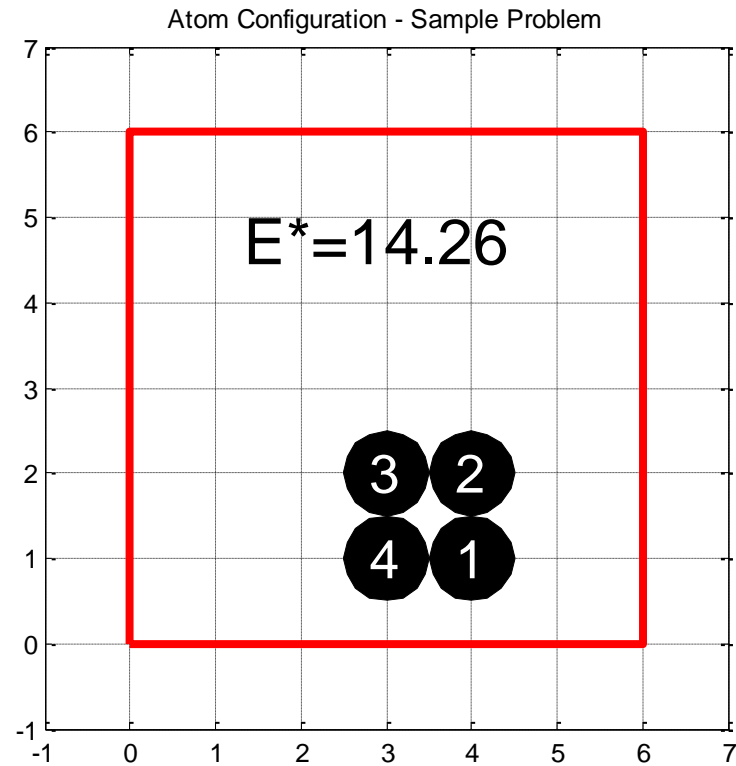
Low gravity   g=0.1

Simulated Annealing

Dilemma

- Cannot compute energy of all configurations !
  - Design space often too large
  - Computation time for a single function evaluation can be large
- Use Metropolis Algorithm, at successively lower temperatures to find low energy states
  - Metropolis: Simulate behavior of a set of atoms in thermal equilibrium (1953)
  - Probability of a configuration existing at T $\rightarrow$ Boltzmann Probability $P(r,T)=\exp(-E(r)/T)$

The SA Algorithm

- **Terminology:**
  - X (or R or Γ) = Design Vector (i.e. Design, Architecture, Configuration)
  - *E* = System Energy (i.e. Objective Function Value)
  - *T* = System Temperature
  - Δ = Difference in System Energy Between Two Design Vectors

- **The Simulated Annealing Algorithm**

  1) Choose a random X_i, select the initial system temperature, and specify the cooling (i.e. annealing) schedule

  2) Evaluate $E(X_i)$ using a simulation model

  3) Perturb X_i to obtain a neighboring Design Vector (X_{i+1})

  4) Evaluate $E(X_{i+1})$ using a simulation model

  5) If $E(X_{i+1}) < E(X_i)$, X_{i+1} is the new current solution

  6) If $E(X_{i+1}) > E(X_i)$, then accept X_{i+1} as the new current solution with a probability $e^{(-\Delta/T)}$ where $\Delta = E(X_{i+1}) - E(X_i)$.

  7) Reduce the system temperature according to the cooling schedule.
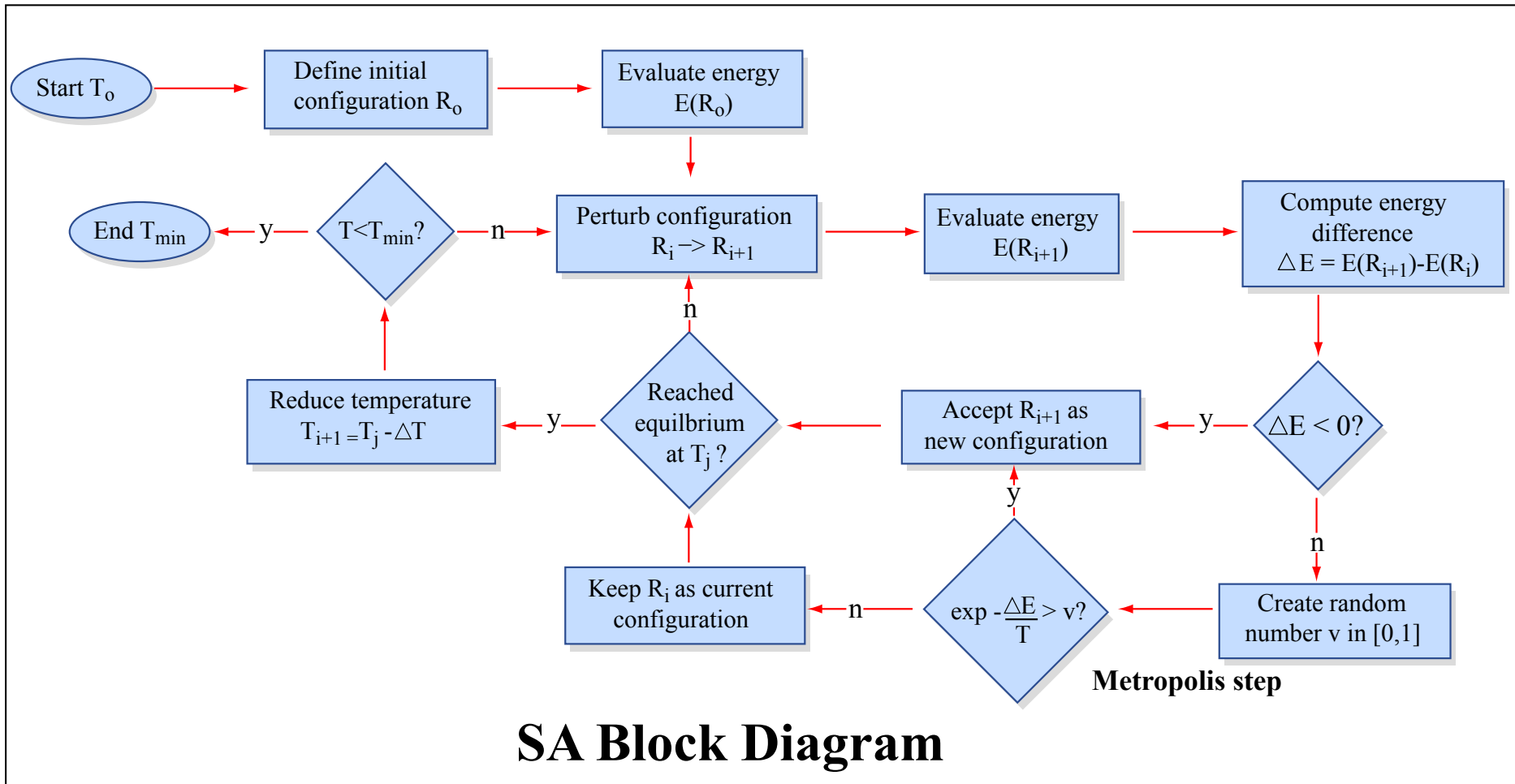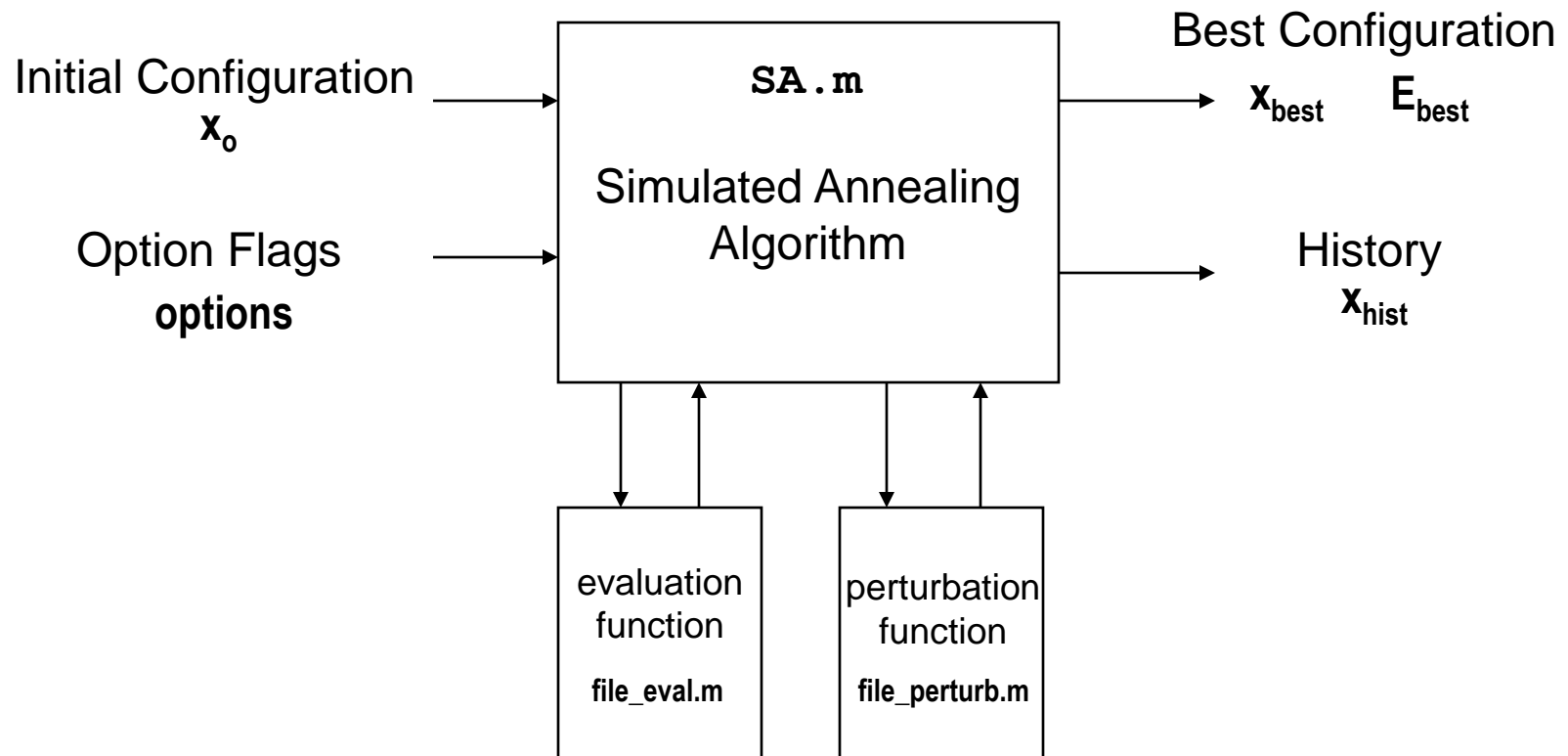
  8) Terminate the algorithm.

SA Block Diagram

SA Block Diagram

Image by MIT OpenCourseWare.

MATLAB Function: `SA.m`

Initial Configuration x_o

Option Flags **options**

SA.m

Simulated Annealing Algorithm

Best Configuration x_{best} E_{best}

History x_{hist}

evaluation function **file_eval.m**

perturbation function **file_perturb.m**

Exponential Cooling

- Typically $(T_1/T_o) \sim 0.7\text{-}0.9$

$$T_{k+1} = \left(\frac{T_1}{T_o} \right)^k T_k$$

Simulated Annealing Evolution
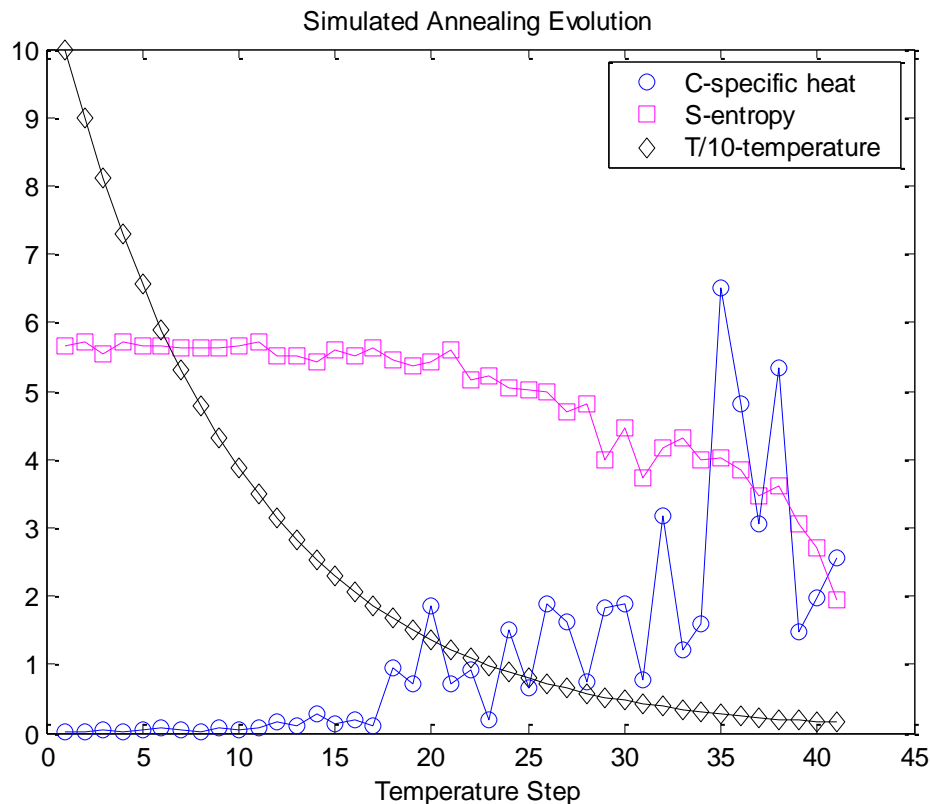
Can also do linear
or step-wise cooling

…

But exponential cooling
often works best.

Key Ingredients for SA

1. A concise description of a configuration (architecture, design, topology) of the system (Design Vector).

2. A random generator of rearrangements of the elements in a configuration (Neighborhoods). This generator encapsulates rules so as to generate only <u>valid</u> configurations. Perturbation function.

3. A quantitative objective function containing the trade-offs that have to be made (Simulation Model and Output Metric(s)). Surrogate for system energy.

4. An annealing schedule of the temperatures and/or the length of times for which the system is to be evolved.

Sample Problems
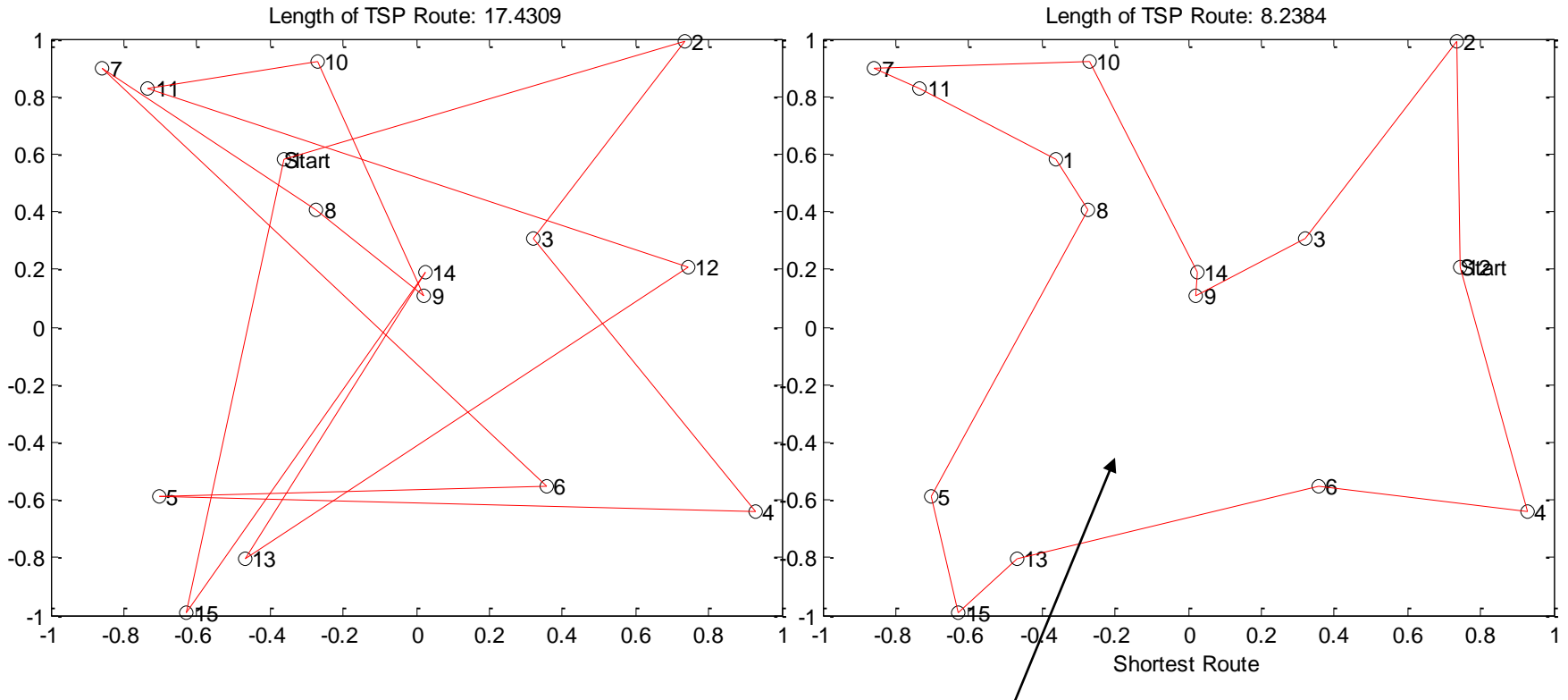
Traveling Salesman Problem

- *N* cities arranged randomly on [-1,1]
- Choose N=15
- SAdemo2.m
- Minimize "cost" of route (<u>length</u>, time,…)
- Visit each city once, return to start city

$$l\left(R\right) = \underbrace{\sum_{i=1}^{N} \sqrt{\sum_{j=1}^{2} \left(x_j\left(R_{i+1}\right) - x_j\left(R_i\right)\right)^2}}_{\text{visit N cities}} + \underbrace{\sqrt{\sum_{j=1}^{2} \left(x_j\left(R_1\right) - x_j\left(R_N\right)\right)^2}}_{\text{return home to first city}}$$

TSP Problem (cont.)

Initial (Random) Route
Length: 17.43

Final (Optimized) Route
Length: 8.24

Result with SA

Structural Optimization

- Define:
  - Design Domain
  - Boundary Conditions
  - Loads
  - Mass constraint
- Subdivide domain
  - N x M design "cells"
  - Cell density ρ=1 or ρ=0
- Where to put material to minimize compliance?
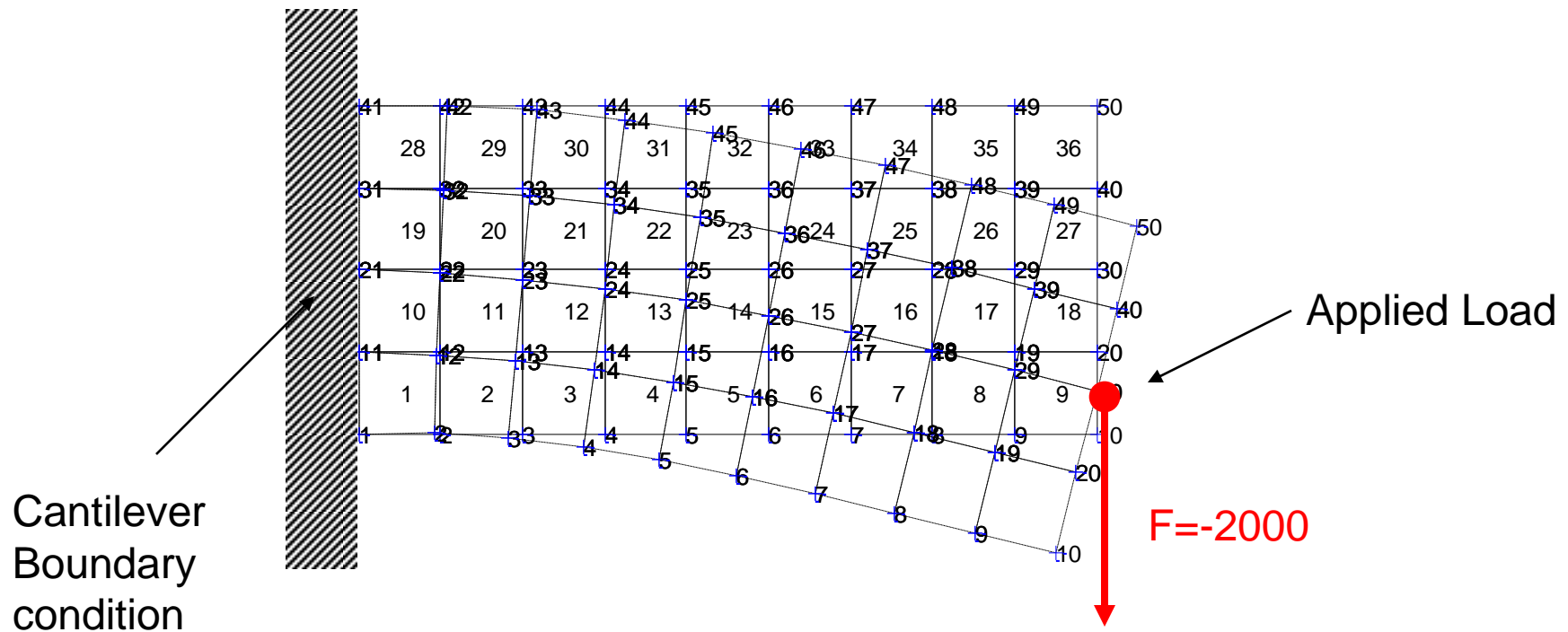
$$\text{find} \quad \rho_i \qquad i = 1,...,N$$

$$\min C = f^T u(\rho_i)$$

$$\text{s.t.} \quad u = K^{-1}f$$

$$\text{s.t.} \quad \sum_{i=1}^{N} V_i \rho_i \leq m_{\max}$$
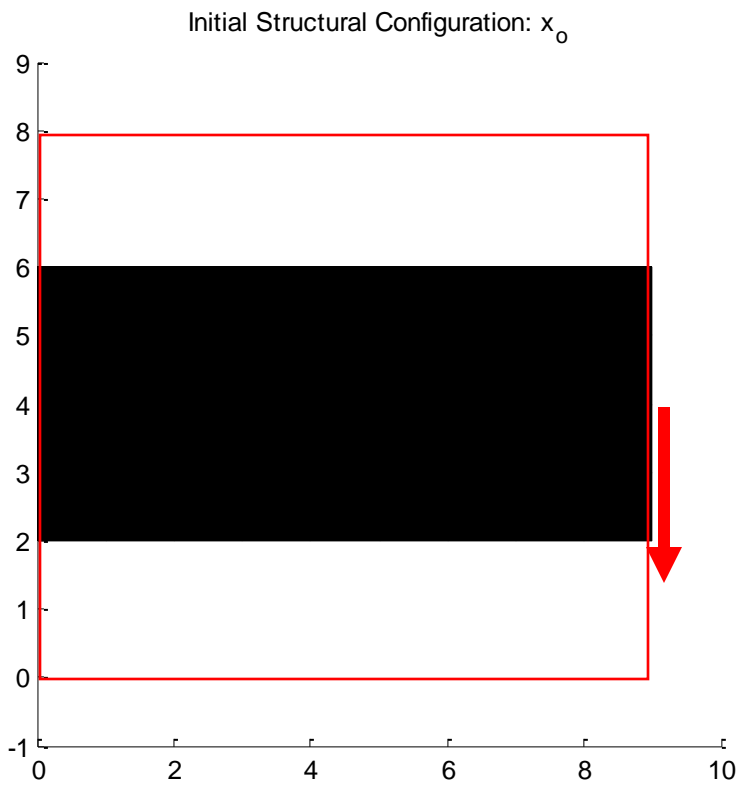
Structural Topology Optimization (II)

"Energy" = strain energy = compliance
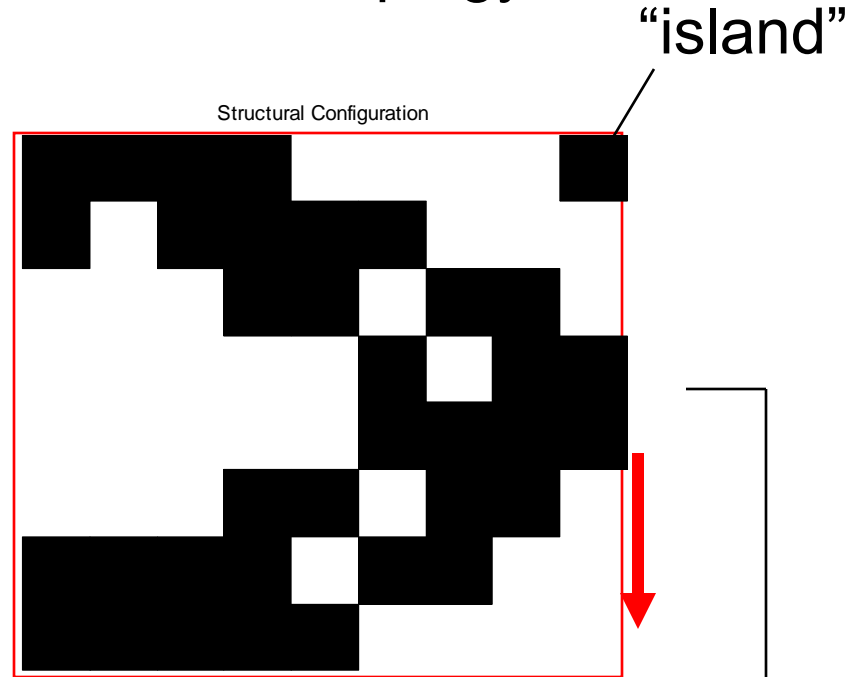Computed via Finite Element Analysis

Cantilever
Boundary
condition

Applied Load

F=-2000

Deformation not drawn to scale

Structural Toplogy Optimization

Initial Structural Toplogy

Initial Structural Configuration: x_o

Compliance C=593.0

"Final" Toplogy

"island"

Structural Configuration

Compliance C=236.68

Not "optimal" – often
need post-processing

Structural Optimization – Convergence Analysis

Boltzmann Distributions

Evolution of
- Entropy, Temperature, Specific Heat

# Premature termination

SA convergence history
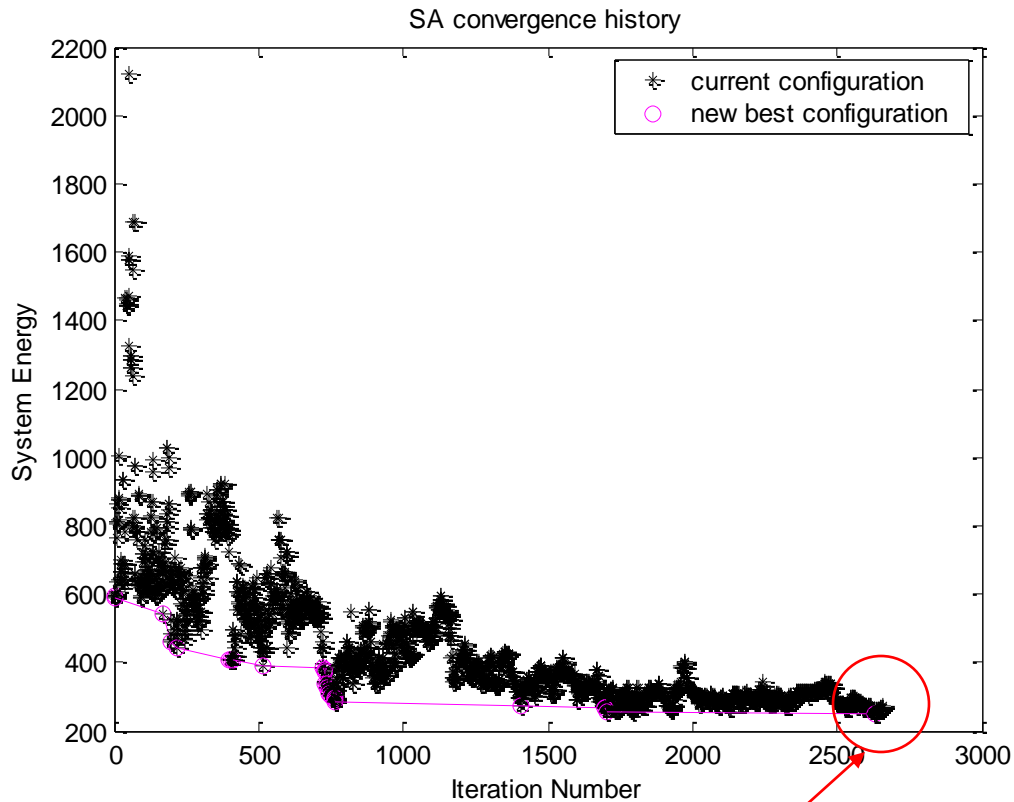
Indicator: Best Configuration found only shortly before Simulated Annealing terminated.
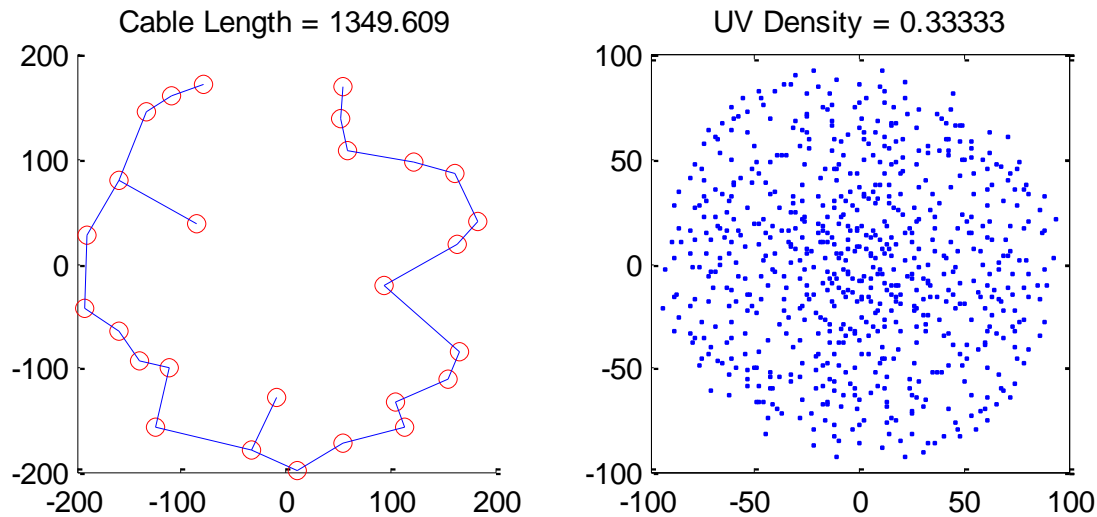
Final Example: Telescope Array Optimization

- Place *N*=27 stations in xy within a 200 km radius
- Minimize UV density metric
- Ideally also minimize cable length

Initial Configuration

Cable Length = 1064.924

UV Density = 0.67236

Optimized Solution

Cable Length = 1349.609

UV Density = 0.33333
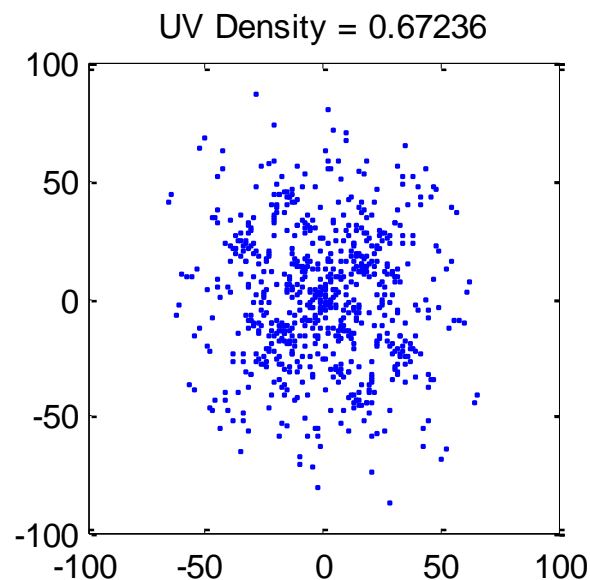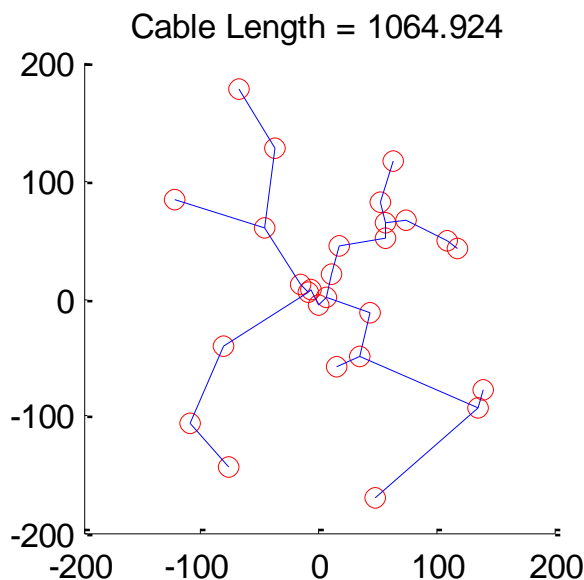
Simulated Annealing

Improved UV density from 0.67 to 0.33

- ## Simulated Annealing transforms the array:
  - Hub-and-Spoke → Circle-with-arms

Cohanim B. E., Hewitt J. N., and de Weck O.L., "The Design of Radio Telescope Array Configurations using Multiobjective Optimization: Imaging Performance versus Cable Length", *The Astrophysical Journal,* Supplement Series, 154, 705-719, October 2004

Summary

Summary: Steps of SA

- **The Simulated Annealing Algorithm**

  1) Choose a random X_i, select the initial system temperature, and outline the cooling (ie. annealing) schedule

  2) Evaluate $E(X_i)$ using a simulation model

  3) Perturb X_i to obtain a neighboring Design Vector (X_{i+1})

  4) Evaluate $E(X_{i+1})$ using a simulation model

  5) If $E(X_{i+1}) < E(X_i)$, X_{i+1} is the new current solution

  6) If $E(X_{i+1}) > E(X_i)$, then accept X_{i+1} as the new current solution with a probability $e^{(-\Delta/T)}$ where $\Delta = E(X_{i+1}) - E(X_i)$.

  7) Reduce the system temperature according to the cooling schedule.

  8) Terminate the algorithm.

Recent Research in SA

- Alternative Cooling Schedules and Termination criteria

- Adaptive Simulated Annealing (ASA) – determines its own cooling schedule

- Hybridization with other Heuristic Search Methods (GA, Tabu Search …)

- Multiobjective Optimization with SA

References

- Cerny, V., "Thermodynamical Approach to the Traveling Salesman Problem: An Efficient Simulation Algorithm", *J. Opt. Theory Appl.*, 45, 1, 41-51, 1985 .

- de Weck O. "System Optimization with Simulated Annealing (SA), Memorandum SA.pdf

- Cohanim B. E., Hewitt J. N., and de Weck O.L., "The Design of Radio Telescope Array Configurations using Multiobjective Optimization: Imaging Performance versus Cable Length", The Astrophysical Journal, Supplement Series, 154, 705-719, October 2004

- Jilla, C.D., and Miller, D.W., "Assessing the Performance of a Heuristic Simulated Annealing Algorithm for the Design of Distributed Satellite Systems," *Acta Astronautica*, Vol. 48, No. 5-12, 2001, pp. 529-543.

- **Kirkpatrick, S., Gelatt, C.D., and Vecchi, M.P., "Optimization by Simulated Annealing," *Science*, Volume 220, Number 4598, 13 May 1983, pp. 671-680.**

- Metropolis,N., A. Rosenbluth, M. Rosenbluth, A. Teller, E. Teller, "Equation of State Calculations by Fast Computing Machines", *J. Chem. Phys.*,21, 6, 1087-1092, 1953.

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