Metaheuristic Optimization

7. Simulated Annealing

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Outline

1. Introduction
2. Metropolis Algorithms
3. Simulated Annealing
4. Temperature Scheduling
5. Implementation
6. Summary

website

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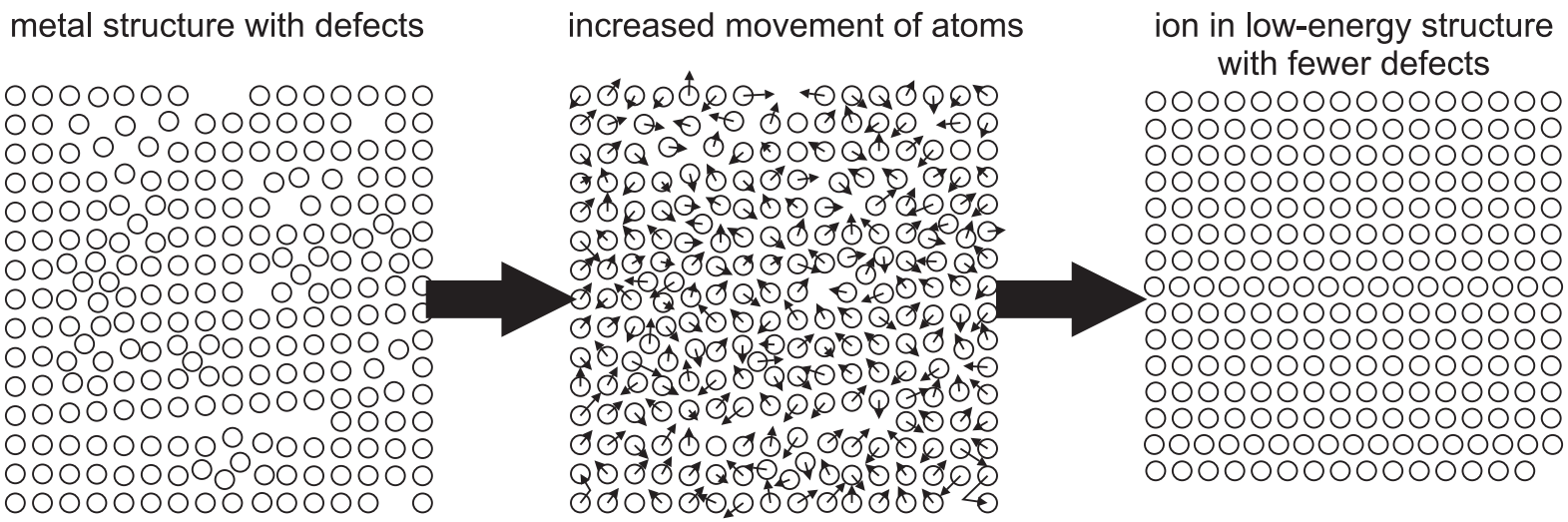
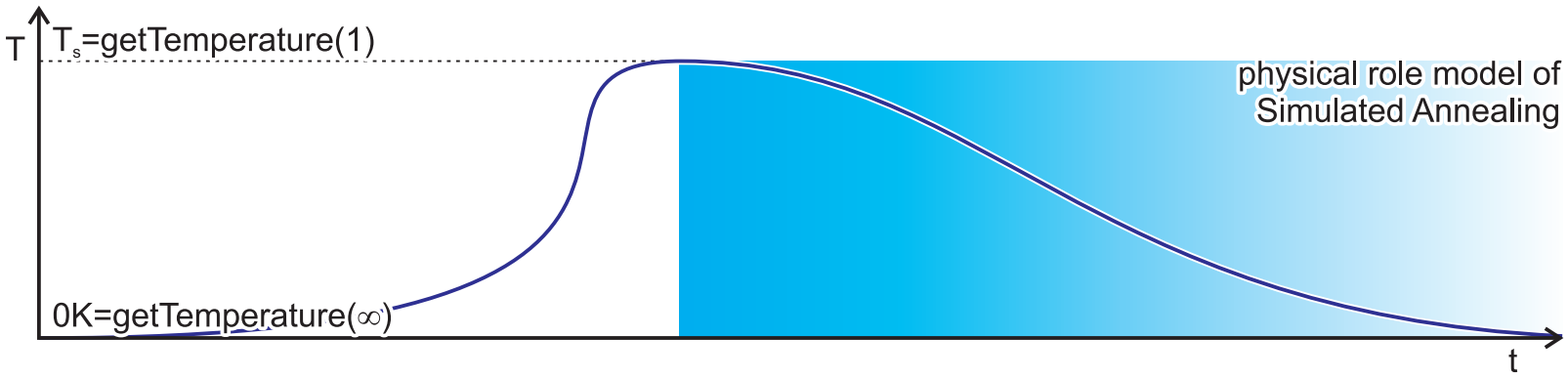
- Due to their movement, ions may temporarily assume positions of high energy
- An initial, brittle crystal structure is transformed to a much better configuration by stepping over good and bad states

Introduction: Annealing





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$$k_b = 1.380650524 * 10^{-27} J/K \text{ is the Boltzmann constant} \quad (1)$$

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- Now we consider a value of E as a macro-state of the system and to each such state, there belong many possible micro-states
- A system at temperature T has the probability $e^{-\frac{E}{k_B * T}}$ to be in a macro state with energy E.
- In other words: The higher the temperature, the higher the chance to be in a high-energy state

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- ⇒ lower risk of premature convergence

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- Temperature T reduced according to a specific schedule over the iterations

$p_{best} \longleftarrow \text{simulatedAnnealing}(f)$

Input: f: the objective function to be minimized
Data: p_{new}: the newly generated individual
Data: p_{cur}: the point currently investigated
Data: T: the temperature of the system which is decreased over time
Data: t: the current time index
Data: ΔE: the energy (objective value) difference of the $p_{cur}.x$ and $p_{new}.x$
Output: p_{best}: the best individual ever discovered

```
begin
    p_cur ⟵ create and evaluate initial solution
    p_best ⟵ p_cur
    t ⟵ 1
    while ¬shouldTerminate do
        p_new ⟵ derive new solution from p_cur
        ΔE ⟵ f(p_new) − f(p_cur)
        if ΔE ≤ 0 then
            p_cur ⟵ p_new
            if f(p_cur.x) < f(p_best.x) then p_best ⟵ p_cur
        else
            T ⟵ getTemperature(t)
            if {randomly from [0,1]} < e^(−ΔE/T) then p_cur ⟵ p_new
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begin
    p_cur.g ⟵ create()
    p_cur.x ⟵ gpm(p_cur.g)
    p_cur.y ⟵ f(p_cur.x)
    p_best ⟵ p_cur
    t ⟵ 0
    while ¬shouldTerminate do
        p_new.g ⟵ mutation(p_cur.g)
        p_new.x ⟵ gpm(p_new.g)
        p_new.y ⟵ f(p_new.x)
        ΔE ⟵ p_new.y − p_cur.y
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- Full algorithm

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Definition (Temperature Schedule)

The temperature schedule defines how the temperature parameter T in the Simulated Annealing process is set. The operator $\mathrm{getTemperature} : \mathbb{N}_1 \mapsto \mathbb{R}^+$ maps the current iteration index t to a (positive) real temperature value T. [12, 13]

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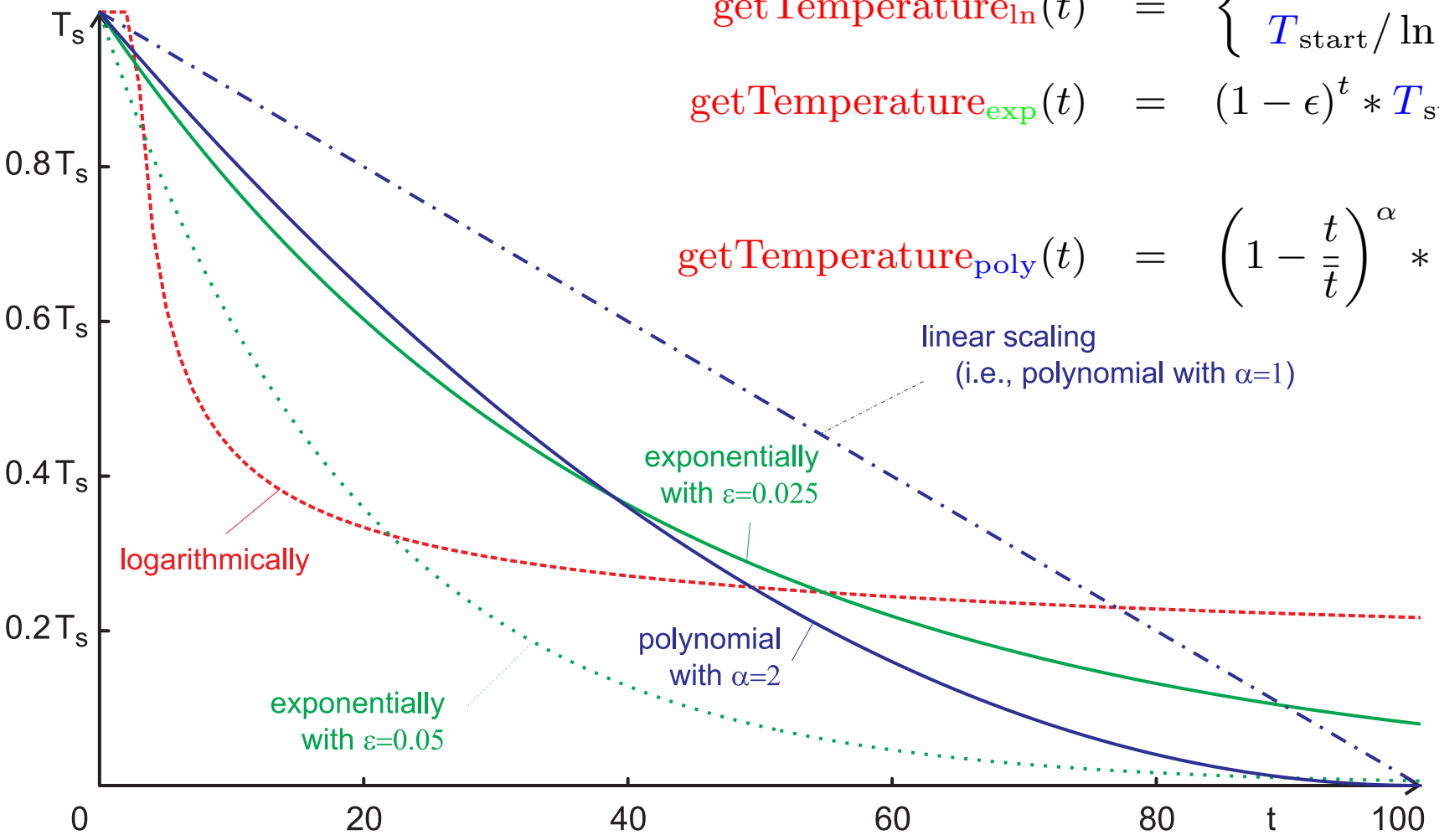
The temperature schedule allows for a smooth transition of SA algorithm behavior from "like Random Walk" (high temperature) to "like hill climbing" (low temperature).

Temperature Scheduling

$$\text{getTemperature}_{\text{ln}}(t) = \begin{cases} T_{\text{start}} & \text{if } t < 3 \\ T_{\text{start}} / \ln t & \text{otherwise} \end{cases}$$

$$\text{getTemperature}_{\text{exp}}(t) = (1-\epsilon)^t * T_{\text{start}}$$

$$\text{getTemperature}_{\text{poly}}(t) = \left(1 - \frac{t}{\bar{t}}\right)^{\alpha} * T_{\text{start}}$$



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- Often: Adjust temperature only every $m \in \mathbb{N}_1$ steps

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- Here: Restarting good in order avoid premature convergence

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Implementation

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- Add a new interface for temperature scheduling
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- Test

From the programmer's perspective, we can say:

Listing: Temperature Schedule getTemperature

```
public interface ITemperatureSchedule {

  public abstract double getTemperature(final int t);
}
```

Listing: Simulated Annealing

```
public class SA<G, X> extends OptimizationAlgorithm<G, X> {
  public Individual<G, X> solve(final IObjectiveFunction<X> f) {
    Individual<G, X> pcur, pnew, pbest;
    double deltaE, T;
    int t;

    pcur = new Individual<>();
    pnew = new Individual<>();
    pbest = new Individual<>();

    t = 1;
    pcur.g = this.nullary.create(this.random);
    pcur.x = this.gpm.gpm(pcur.g);
    pcur.v = f.compute(pcur.x);
    pbest.assign(pcur);

    while (!(this.termination.shouldTerminate())) {
      pnew.g = this.unary.mutate(pcur.g, this.random);
      pnew.x = this.gpm.gpm(pnew.g);
      pnew.v = f.compute(pnew.x);
      deltaE = (pnew.v - pcur.v);

      if (deltaE <= 0d) {
        pcur.assign(pnew);
        if (pnew.v < pbest.v) {
          pbest.assign(pnew);
        }
      } else {
        T = this.temperature.getTemperature(t);
        if (this.random.nextDouble() < Math.exp(-deltaE / T)) {
          pcur.assign(pnew);
        }
      }
      t++;
    }
    return pbest;
  }
}
```

The Logarithmic Temperature Schedule

Listing: The Logarithmic Temperature Schedule

```
public class Logarithmic implements ITemperatureSchedule {
  public double getTemperature(final int t) {
    if (t < 3) {
      return this.Ts;
    }
    return (this.Ts / Math.log(t));
  }
}
```

The Exponential Temperature Schedule

Listing: The Exponential Temperature Schedule

```
public class Exponential implements ITemperatureSchedule {
  public double getTemperature(final int t) {
    return (this.Ts * Math.pow((1d - this.epsilon), t));
  }
}
```

The Polynomial Temperature Schedule

Listing: The Polynomial Temperature Schedule

```
public class Polynomial implements ITemperatureSchedule {
  public double getTemperature(final int t) {
    return (this.Ts * Math.pow(Math.max(0d, (1d - (t / this.tmax))),//
        this.alpha));
  }
}
```

Section Outline

1. Introduction
2. Metropolis Algorithms
3. Simulated Annealing
4. Temperature Scheduling
5. Implementation
6. Summary

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- Annealing is a physical process in metallurgy where low-energy configurations are found

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Summary

- Annealing is a physical process in metallurgy where low-energy configurations are found
- This process is simulated with the Metropolis algorithm
- which serves as role model for an optimization algorithm: simulated annealing
- Different temperature schedules
- Convergence to global optimum is guaranteed for many problems and logarithmic schedules ... but very slow
- Simulated quenching is faster but loses guaranteed optimality

谢谢

Thank you

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Caspar David Friedrich, “Der Wanderer über dem Nebelmeer”, 1818
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