A Diagnostic Smoke Test for Simulated Annealing in 2D Circle Packing

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1 Purpose and Scope

This report documents a *diagnostic smoke run* of a correctness-first simulated annealing (SA) implementation for packing identical circles in a square container. The goal of the run is not optimality or performance, but **observability**: to verify that the algorithm behaves consistently with theoretical expectations and to understand how temperature, proposals, and penalties interact over time.

All quantities shown here are produced automatically by the codebase, including per-step logging and post-processing plots.

2 Problem Setup

We consider packing N identical circles of radius r in a square container of side length L. A configuration is given by

$$X = \{x_i \in \mathbb{R}^2 : i = 1, \ldots, N\}.$$

The total energy is

$$E(X, L) = E_{\text{pair}}(X) + E_{\text{wall}}(X, L) + \alpha L,$$

where E_{pair} penalizes overlaps and E_{wall} penalizes boundary violations. In this baseline run, L is fixed and $\alpha = 0$.

2.1 Run Parameters

The smoke run reported here uses:

Number of circles	$N = 20$
Circle radius	$r = 1.0$
Box side length	$L = 20.0$
Initial temperature	$T_0 = 2.0$
Cooling factor	$\gamma = 0.99995$
Number of steps	$n_{\text{steps}} = 8 \times 10^5$
Proposal scale	$\sigma = 0.30$
Random seed	123

The run is designed to complete in under five minutes on typical hardware.

3 Initial Conditions

3.1 Initial Position

The initial configuration X_0 is generated randomly using a seeded pseudo-random number generator.

If $L - 2r > 0$, each coordinate is sampled independently from the interior window:

$$x_i \sim \text{Uniform}(r, L - r), \qquad y_i \sim \text{Uniform}(r, L - r).$$

Otherwise (degenerate case), sampling falls back to

$$x_i, y_i \sim \text{Uniform}(0, L).$$

Thus, the initialization is **uniform, interior, and deterministic** given the seed.

3.2 Initial Box Length

The box side length is set by the input parameter L and remains fixed throughout the run. For this experiment,

$$L = 20.0.$$

No dynamic resizing of the container is performed in this baseline.

4 Annealing Schedule and Runtime

4.1 Algorithmic Duration

The algorithm executes exactly n_{steps} Metropolis proposals. In this run,

$$n_{\text{steps}} = 8 \times 10^5.$$

4.2 Computational Cost

Each proposal updates exactly one circle. The incremental energy computation scales as

$$\mathcal{O}(N),$$

so the total computational work scales approximately as

$$\mathcal{O}(n_{\text{steps}} \cdot N).$$

4.3 Cooling Schedule

A geometric cooling schedule is used:

$$T_{t+1} = \gamma T_t, \qquad T_t = T_0 \gamma^t.$$

For this run,

$$T_0 = 2.0, \qquad \gamma = 0.99995.$$

The temperature half-life is

$$t_{1/2} = \frac{\ln(1/2)}{\ln(\gamma)} \approx 13{,}860 \text{ steps},$$

which yields a slow, steady cooling over the duration of the run.

5 Logged Quantities and Diagnostics

At every Metropolis step, the following quantities are logged:

- step index,
- total energy E,
- temperature T,
- pair overlap energy E_{pair},
- wall penalty energy E_{wall},
- acceptance indicator (0/1),
- index of the proposed circle.

This full-resolution logging enables detailed post-hoc analysis.

6 Results and Plots

6.1 Energy, Temperature, Acceptance, and Penalties

Figure 1 shows four diagnostic panels side by side:

1. Total energy and best-so-far energy versus step.
2. Temperature versus step (log scale).
3. Rolling acceptance rate.
4. Pair and wall energy components versus step.

As expected:

- E_{pair} drops rapidly early, indicating resolution of overlaps.
- E_{wall} reflects boundary interactions and stabilizes later.
- The total energy decreases monotonically in its best-so-far envelope.
- The acceptance rate decreases as temperature cools.

6.2 Energy Change Distribution

Figure 2 shows the distribution of

$$\Delta E_t = E(t) - E(t-1).$$

Early in the run, the distribution is broad, while late in the run it concentrates near zero, reflecting freezing of the dynamics.

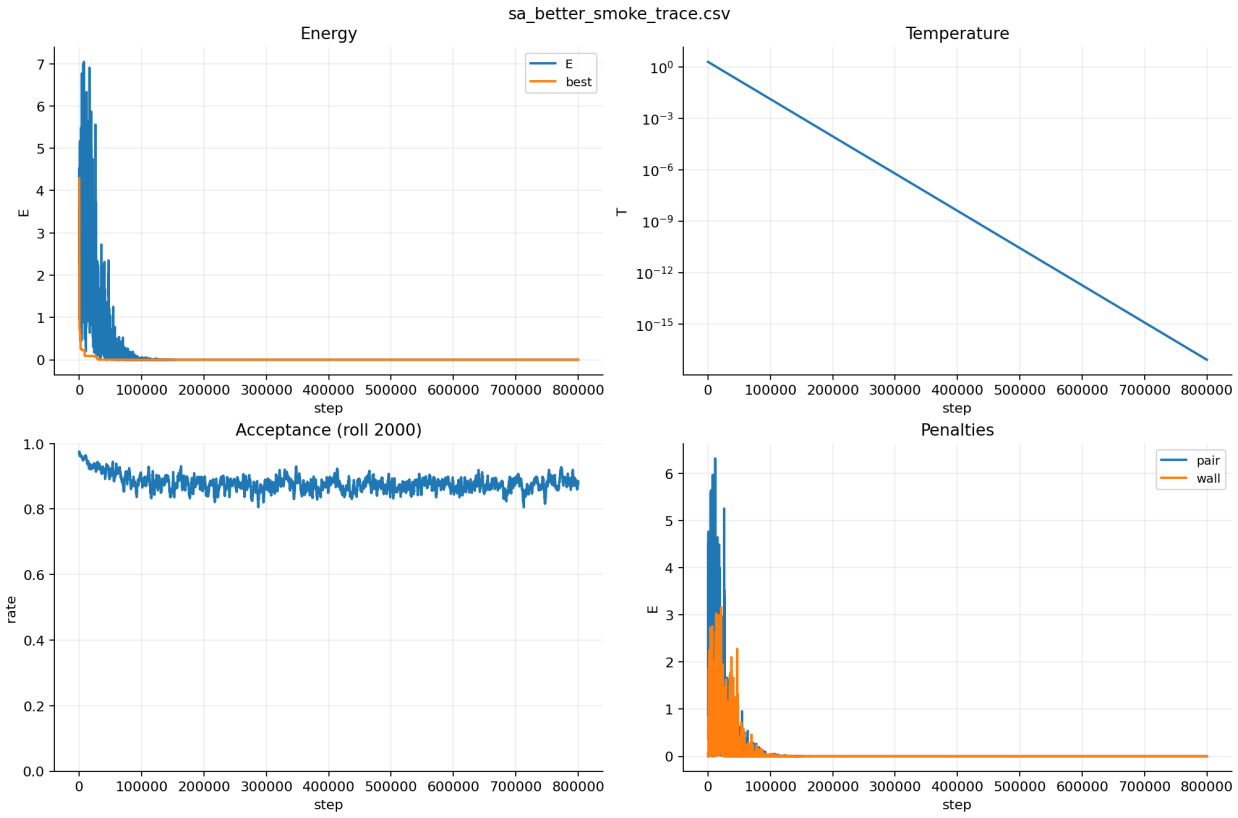

Figure 1: Main diagnostic panels for the simulated annealing run.

6.3 Moved Index Histogram

Figure 3 shows the histogram of proposed circle indices. The distribution is approximately uniform, confirming unbiased selection.

7 Role of Temperature

Temperature affects *only* the acceptance of uphill moves. For $\Delta E > 0$,

$$\mathbb{P}(\text{accept}) = \exp(-\Delta E/T).$$

Thus:

- High T: frequent uphill acceptance $\Rightarrow$ exploration.
- Low T: rare uphill acceptance $\Rightarrow$ exploitation and freezing.

Importantly, temperature does *not* modify the proposal distribution. Proposals are always drawn from

$$\delta \sim \mathcal{N}(0, \sigma^2 I),$$

with fixed σ. Temperature acts as a probabilistic filter on these proposals.

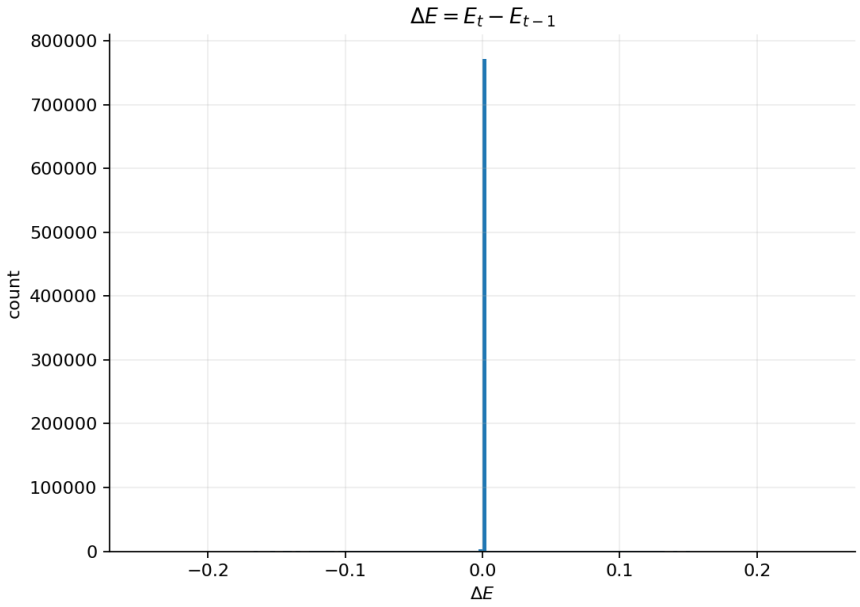

Figure 2: Distribution of energy changes ΔE.

8 Discussion and Recommendations

With aggressive cooling (e.g. $\gamma = 0.999$), temperature halves quickly, and the algorithm becomes greedy early. The slower cooling used here provides better separation between exploration and exploitation phases and produces more interpretable diagnostics.

Possible next steps include:

- adaptive proposal scaling,
- dynamic logging stride,
- joint optimization of (X, L),
- incremental logging of ΔE.

9 Conclusion

This smoke run confirms that the simulated annealing implementation behaves consistently with theoretical expectations. The instrumentation allows direct interpretation of geometric and stochastic effects, providing a solid foundation for further optimization and scaling.

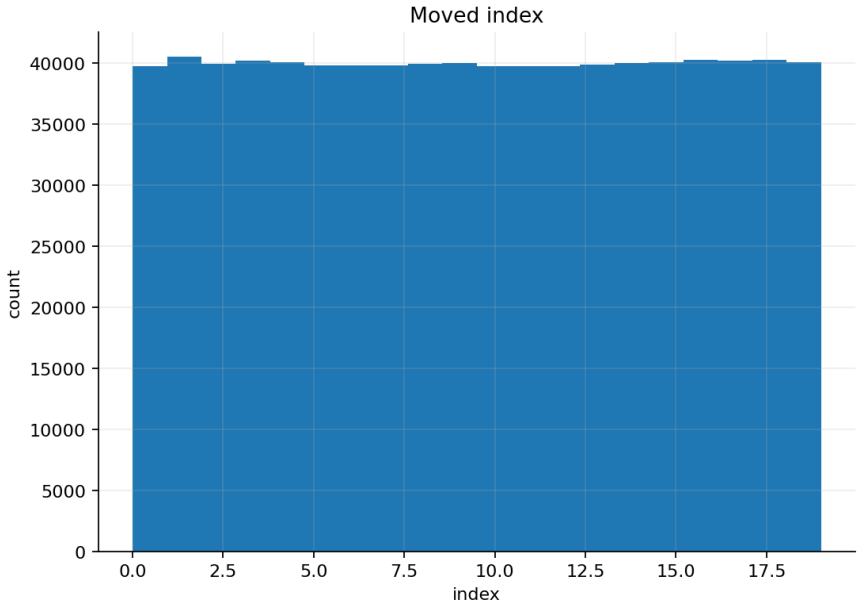

Figure 3: Histogram of moved circle indices.