HPC Simulated Annealing for Non-Convex Polygon Packing in a Square

Bracketing, Bisection Refinement, Time-Limited Shrink Polish, and Sweep Diagnostics

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The Shape We Pack

Agenda

1. Problem and constraints
2. Geometry model: triangulation + SAT + broad-phase rejects
3. Energy function, feasibility, and SA moves
4. Outer optimizer: bracketing + bisection
5. Time-limited polish: adaptive shrink search + checkpoints
6. HPC reliability: determinism, file safety, GLIBC considerations
7. Sweep diagnostics: density, boundary effects, disorder statistics
8. Best-solution visuals

Problem Statement

Goal. Pack N identical copies of a fixed **non-convex** polygon $P \subset \mathbb{R}^2$ into a square of side length L.

Decision variables (per instance $i = 1, \ldots, N$):

$$\left(c_x^{(i)},\, c_y^{(i)},\, \theta^{(i)} \right) \in \mathbb{R}^2 \times [0, 2\pi)$$

where $(c_x^{(i)}, c_y^{(i)})$ is translation and $\theta^{(i)}$ is rotation.

Constraints.

- **Non-overlap:** interiors of instances are disjoint.
- **Containment:** each polygon lies inside the square $[-L/2, L/2]^2$.

Objective. Minimize L (tightest feasible packing).

A Provable Lower Bound (Area Bound)

Let $\mathrm{area}(P)$ be the polygon area. Then any feasible packing must satisfy:

$$L^2 \;\geq\; N \cdot \mathrm{area}(P) \quad \Rightarrow \quad L \;\geq\; \sqrt{N\,\mathrm{area}(P)}.$$

In code, we keep a strictly provably infeasible threshold:

$$L_{\text{area}} = \sqrt{N\,\mathrm{area}(P)}, \qquad L_{\text{area-infeas}} = (1-\varepsilon)\,L_{\text{area}}.$$

Interpretation. If $L \leq L_{\text{area-infeas}}$, the instance is **provably infeasible** (no need to run SA).

Geometry Model: Triangulation + SAT

We represent the non-convex polygon P by:

- A fixed vertex list $\{v_k\}_{k=1}^{N_V}$ in local coordinates.
- A fixed triangulation $\{\Delta_t\}_{t=1}^{N_T}$, each triangle uses indices into the vertex list.

Each instance i produces world vertices:

$$w_k^{(i)} = R(\theta^{(i)})\, v_k + \begin{bmatrix} c_x^{(i)} \\ c_y^{(i)} \end{bmatrix}.$$

Collision test between instances (i, j):

1. Broad-phase AABB overlap
2. Broad-phase bounding-circle reject
3. Narrow-phase triangle-triangle SAT for all (t_a, t_b)

Broad-Phase Acceleration

AABB reject. If axis-aligned bounding boxes do not overlap, polygons cannot overlap.

Bounding-circle reject. Precompute base radius r:

$$r = \max_k \|v_k\|_2.$$

If centers are far:

$$\|c^{(i)} - c^{(j)}\|_2 > 2r \quad \Rightarrow \quad \text{no overlap.}$$

Uniform grid (spatial hashing). Each instance belongs to one grid cell; collision checks only consider neighbor cells within a radius based on $2r$.

Outcome. Pairwise overlap checks scale with *local neighborhood* interactions rather than $O(N^2)$ in practice.

Containment Penalty via AABB

Containment is enforced through an **outside penalty** computed from AABB vs. square:

$$\mathrm{out}_i(L) = \sum_{\text{violations}} d^2$$

where d is how far the AABB exceeds $\pm L/2$ in any direction.

Benefit. Cheap to compute, robust, and effective when combined with increased penalty weights in Phase B.

Energy Function and Feasibility Metric

We separate **energy** (for SA acceptance) from **feasibility** (for outer logic).

Totals:

$$\mathrm{ov}(L) = \sum_{i<j} \mathrm{overlap\_penalty}(i,j), \qquad \mathrm{out}(L) = \sum_{i} \mathrm{outside\_penalty}(i).$$

Energy (SA at fixed L):

$$\mathcal{E} = \lambda\,\mathrm{ov} + \mu\,\mathrm{out}$$

(with weights scheduled by phase).

Feasibility metric:

$$\mathrm{feas} = \mathrm{ov} + \mathrm{out}.$$

We declare "feasible" if $\mathrm{feas} \le \tau$ for a small tolerance τ and L is not area-provably infeasible.

Move Set and Incremental Updates

Each SA iteration chooses a random index k and applies one of:

- **Reinsert (small probability):** randomize (c_x, c_y, θ) uniformly.
- **Local jitter:** $(c_x, c_y) \leftarrow (c_x, c_y) + \Delta$, $\Delta \sim \mathrm{Unif}([-s, s]^2)$.
- **Rotation mix:** with probability p_{rot}, $\theta \leftarrow \theta + \Delta\theta$.

Incremental bookkeeping. Only terms involving instance k are recomputed:

$$\mathrm{ov} \leftarrow \mathrm{ov} + (\mathrm{ov}_k^{\mathrm{new}} - \mathrm{ov}_k^{\mathrm{old}}), \qquad \mathrm{out} \leftarrow \mathrm{out} + (\mathrm{out}_k^{\mathrm{new}} - \mathrm{out}_k^{\mathrm{old}}).$$

Outcome. Fast inner loop; suitable for HPC sweeps over many N.

Two-Phase SA Schedule

We use two sequential phases at fixed L:

Phase A (Explore).

- Higher temperature $T_{\text{start}} \to T_{\text{end}}$
- Larger step sizes
- Moderate penalties (λ, μ)
- Purpose: escape poor initializations and reduce gross overlaps/outside

Phase B (Enforce).

- Lower temperatures
- Smaller step sizes
- **Penalty ramp:** $(\lambda, \mu) \leftarrow \min((\lambda, \mu) \cdot \rho,\ (\lambda_{\max}, \mu_{\max}))$
- Purpose: aggressively drive $\mathrm{feas} \to 0$

SA Acceptance Rule

Given current energy $\mathcal{E}$ and proposed energy $\mathcal{E}'$, accept with:

$$\Delta\mathcal{E} = \mathcal{E}' - \mathcal{E}, \qquad \mathbb{P}(\text{accept}) = \begin{cases} 1, & \Delta\mathcal{E} \le 0, \\ \exp(-\Delta\mathcal{E}/T), & \Delta\mathcal{E} > 0. \end{cases}$$

We track the best feasibility configuration during the run:

$$\text{feas}_{\text{min}} = \min_{t} \text{feas}(t),$$

and restore to that best configuration at the end of each trial.

Simulated Annealing at Fixed L (Clean Skeleton)

State

$$x = \{(c_x^{(i)}, c_y^{(i)}, \theta^{(i)})\}_{i=1}^{N}$$

Energy and Feasibility

$$\mathcal{E}(x; L) = \lambda \operatorname{ov}(x) + \mu \operatorname{out}(x; L), \qquad \operatorname{feas}(x; L) = \operatorname{ov}(x) + \operatorname{out}(x; L)$$

Algorithm Skeleton

1. Initialize x (grid init or warm-start)
2. Phase A (explore): larger moves, higher temperature
3. Phase B (enforce): smaller moves, ramp penalties
4. Track best snapshot (minimum feas) and return it

Outer Loop Overview

We minimize L via:

1. **Initialize** L from a grid layout (near-square arrangement).
2. **Bracketing:** shrink until infeasible (or grow until feasible) to find $[L_{\text{low}}, L_{\text{high}}]$.
3. **Bisection:** refine the bracket to a tight feasible L.
4. **Polish:** time-limited stochastic descent to shrink further.

Reliability constraints. The area bound prevents invalid brackets; best configurations are carried across L updates by scaling warm-starts.

Bisection Refinement

Given $L_{\text{low}} < L_{\text{high}}$:

$$L_{\text{mid}} = \tfrac{1}{2}(L_{\text{low}} + L_{\text{high}}).$$

If $L_{\text{mid}} \leq L_{\text{area-infeas}}$: mark infeasible without SA.

Else:

- Warm-start by scaling best-feasible configuration from L_{high} to L_{mid}.
- Run bounded SA trials at L_{mid}.
- If feasible: $L_{\text{high}} \leftarrow L_{\text{mid}}$; else $L_{\text{low}} \leftarrow L_{\text{mid}}$.

After k steps, bracket width shrinks by 2^{-k}.

Polish Stage: Adaptive Shrink Search

After bisection, we have a strong feasible configuration at $L^\star$.

Attempt a shrink:

$$L_{\text{try}} = L^\star(1 - \epsilon)$$

Scale positions, then run a few SA trials.

Adaptive control. Tune ϵ based on recent success rate (stochastic descent with backoff) until time limit is reached.

Time Limit, Checkpoints, and SIGTERM

Time-limited polish. We cap polish runtime (e.g., 900s) to guarantee completion in Slurm arrays.

Periodic checkpoints (every Δt seconds):

- `csv/<prefix>_checkpoint_Nxxx.csv`
- `img/<prefix>_checkpoint_Nxxx.svg`

SIGTERM handling. Near walltime Slurm sends SIGTERM; the handler:

- flushes **best snapshot** to best and checkpoint files,
- exits cleanly.

Outcome. Even canceled jobs produce usable artifacts.

HPC Engineering: Determinism and File Safety

Deterministic seeds. Each trial seed is derived from:

$$\text{seed} = f(\text{base\_seed},\ \text{run\_id},\ \text{trial\_id})$$

(e.g., SplitMix64 diffusion) for reproducibility across array jobs.

Unique output prefixes.

$$\texttt{out\_prefix} = \texttt{N\{N\}\_job\{job\}\_task\{task\}}$$

prevents file collisions under concurrency.

Build environment. Compile on compute nodes (or use cluster toolchain) to avoid GLIBC mismatch between login/desktop and compute nodes.

Complexity Notes and Practical Performance

Worst case. Collision evaluation can be heavy, but practice is improved by:

- grid neighbor enumeration (local pairs),
- AABB + bounding-circle rejects (broad phase),
- small fixed triangulation size (N_T constant),
- incremental updates per move (only one instance changes).

Scaling expectation. Runtime grows with local density and neighbor interactions, typically milder than $O(N^2)$.

Overnight HPC Sweep: Execution Summary

What Was Run

A Slurm job array solved **200 independent packing problems**, one per $N = 1, \ldots, 200$, using identical solver logic and fixed per-task budgets.

Resource Budget

- Up to **20 tasks in parallel** (`#SBATCH --array=1-200%20`)
- **30 minutes wall time per task** (`#SBATCH --time=00:30:00`)
- 1 CPU core, 2 GB memory per task

Time Allocation Within Each Task

- **Bracketing + bisection:** bounded SA trials (designed to always finish)
- **Polish stage:** time-limited to **12 minutes**
- **Checkpoints:** every 3 minutes during polish
- **Termination safety:** SIGTERM handler flushes best artifacts before exit

Parallelization Model

Type of Parallelism

Embarrassingly parallel parameter sweep. Each value of N is solved independently:

$$\text{Task } N \quad \longleftrightarrow \quad \text{one SLURM array element.}$$

Why This Scales Well

- No inter-task communication or synchronization
- No MPI overhead; pure throughput scaling
- Fault isolation: failure at one N does not affect others

Scheduling Benefits

- Slurm load-balances variable runtimes across N
- Concurrency cap prevents queue flooding
- Natural extension to longer per-N runs or replicated runs per N

Reproducibility Under Parallel Execution

Deterministic Seeding

Each task uses a fixed base seed combined with:

$$\text{seed} = f(\text{base seed},\ N,\ \text{trial id}),$$

ensuring reproducibility regardless of execution order or node placement.

File Safety

- Unique output prefixes: `N{N}_job{job}_task{task}`
- No collisions under concurrent tasks
- Safe output on shared filesystems

Reliability

- SIGTERM delivered before wall time (buffer) to flush artifacts
- Periodic checkpoints reduce risk of losing progress

Sweep Outputs and Aggregation

For each N, the code writes:

- `img/<prefix>_best_Nxxx.svg` and `csv/<prefix>_best_polys_Nxxx.csv`
- `img/<prefix>_checkpoint_Nxxx.svg` and `csv/<prefix>_checkpoint_Nxxx.csv`

A sweep analysis script aggregates all best CSVs into:

- `analysis/summary.csv` (one row per N)
- `analysis/plots/*.png` (diagnostic graphs)

These plots quantify **how tight** the packing is and **why** larger N can become loose.

Key Packing Quality Metrics

Let $\mathrm{area}(P)$ be polygon area and $L(N)$ be best feasible side length for size N.

Density (primary):

$$\rho(N) = \frac{N\,\mathrm{area}(P)}{L(N)^2} \qquad \text{(higher is better)}$$

Empty area (slack):

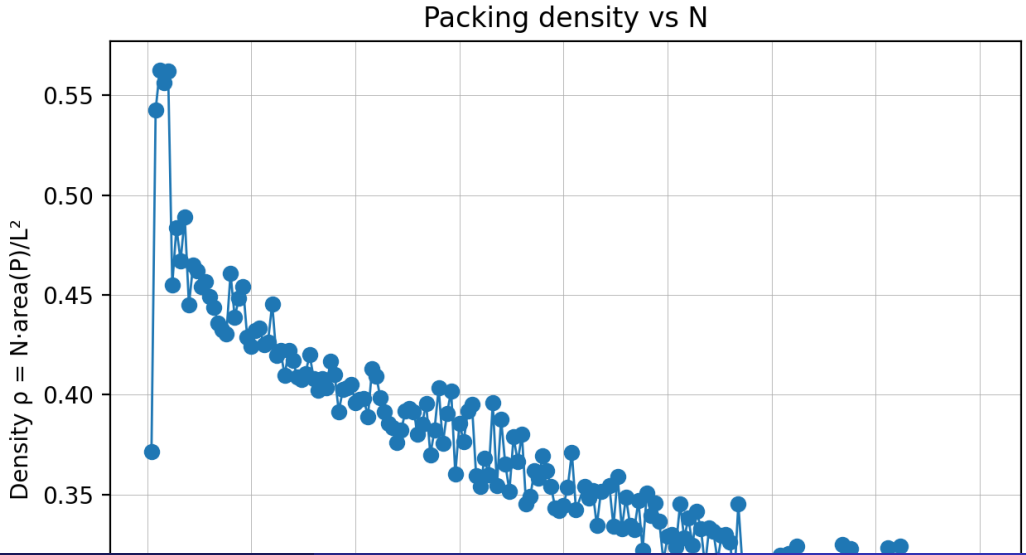
$$\Delta A(N) = L(N)^2 - N\,\mathrm{area}(P)$$

Boundary fraction (boundary waste proxy): fraction of centers within distance kr of the square boundary, where r is the polygon bounding radius.

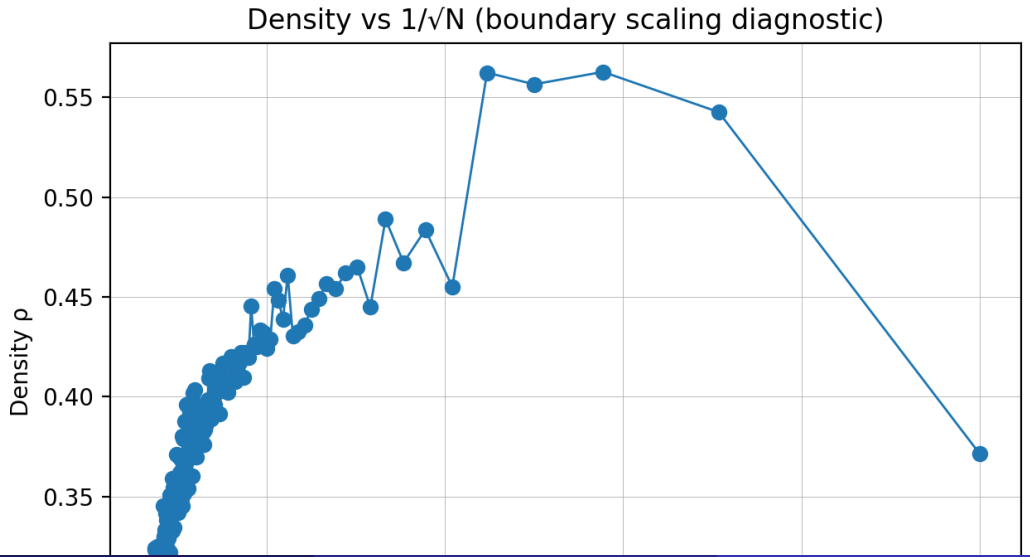
Structure/disorder:

- nearest-neighbor distance statistics (mean / std),
- orientation entropy of $\{\theta_i\}$ (high entropy $\Rightarrow$ amorphous).

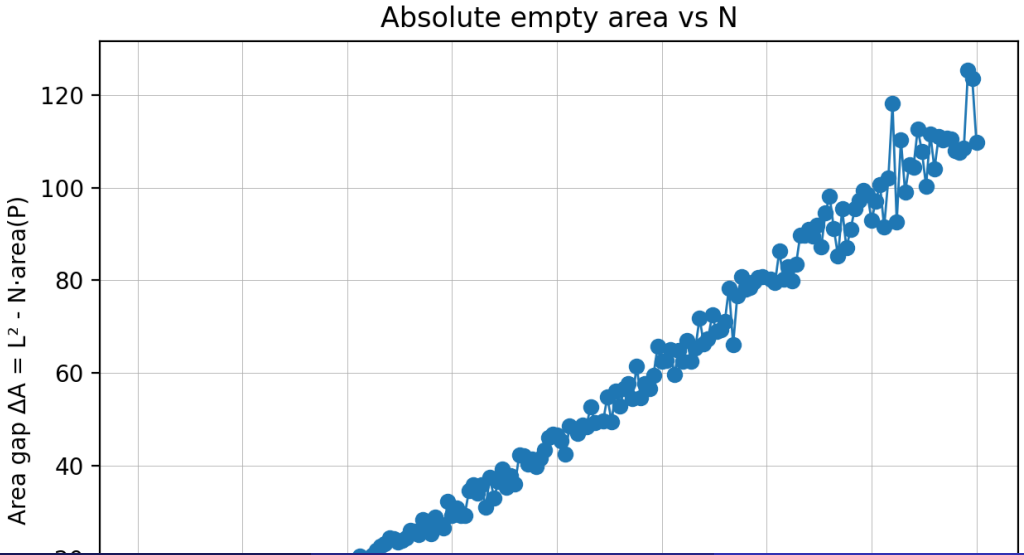
Density vs N



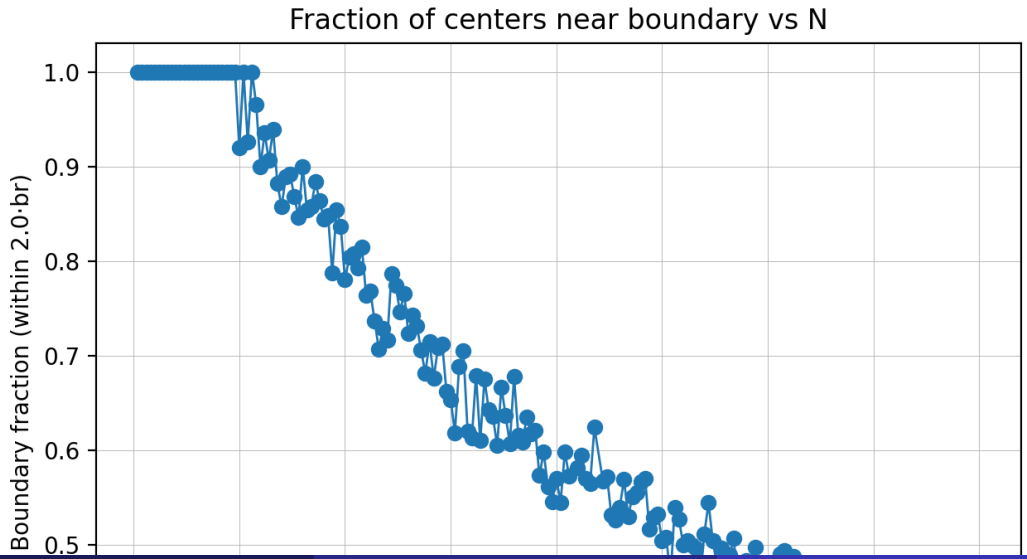
Density vs $1/\sqrt{N}$ (Boundary Scaling Diagnostic)



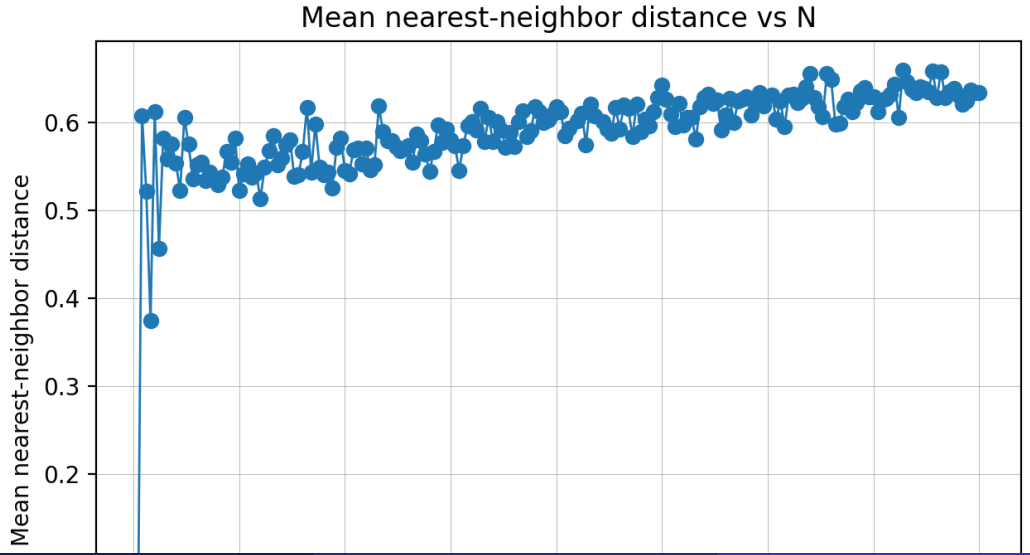
Empty Area (Slack) vs N



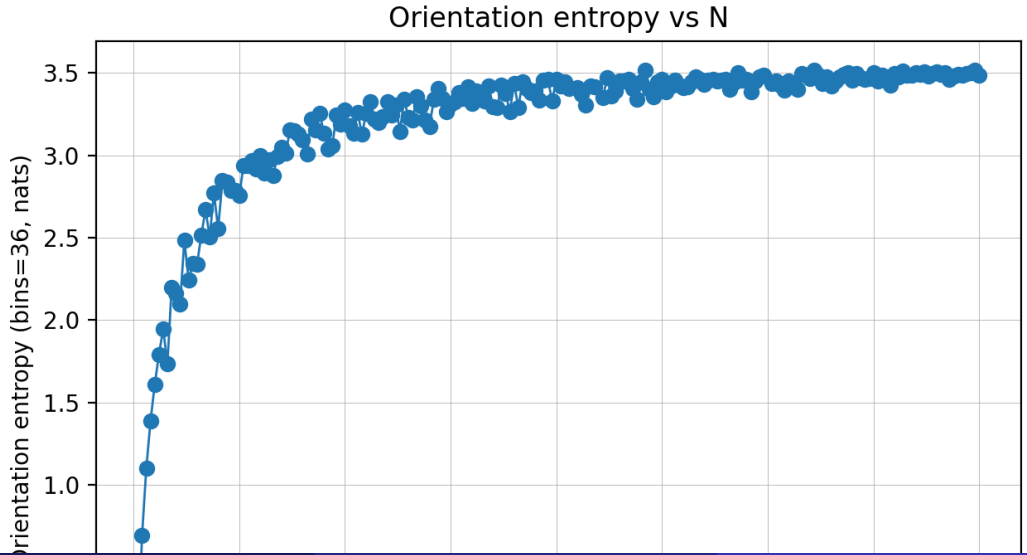
Boundary Fraction vs N



Nearest-Neighbor Spacing vs N



Orientation Entropy vs N



Interpreting the Diagnostics

Case A: boundary-limited (good interior, bad boundary).

- density vs $1/\sqrt{N}$ approximately linear,
- interior spacing stable, but boundary fraction high.

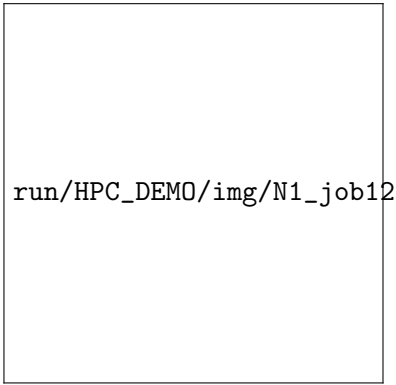
Response: warm-start from a periodic tiling; fit near-square patches; boundary-aware refinement.

Case B: motif failure (interior also loose).

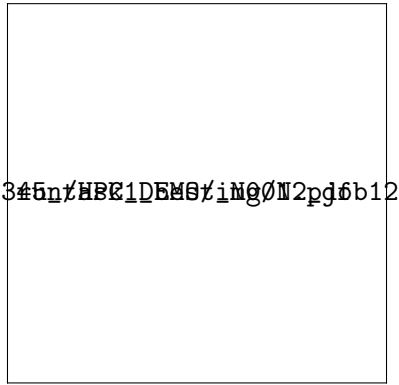
- density flattens too low,
- NN mean grows and orientation entropy remains high.

Response: discover small periodic motifs (periodic boundary SA), then tile; add structured moves / templates.

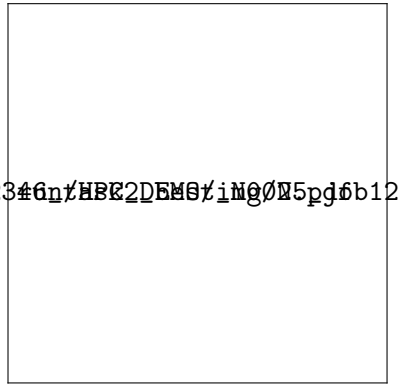
Best Solutions Across N (Small)



$N = 1$

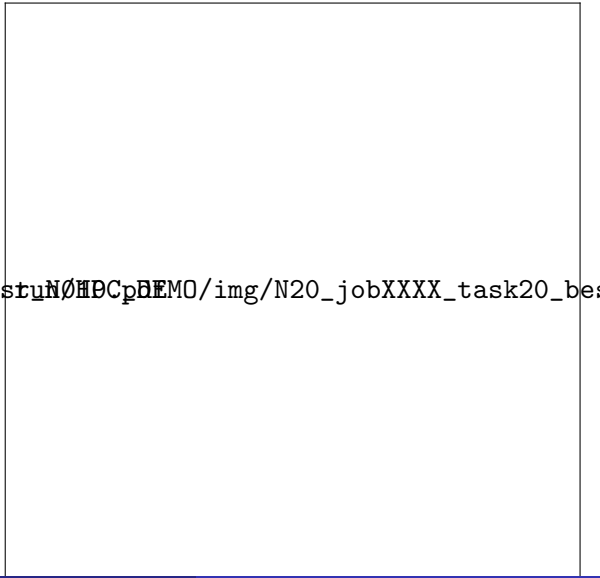


$N = 2$



$N = 5$

Best Solutions Across N (Medium)



Best Solutions Across N (Large)

Best Solution at the Largest Studied N

run/HPC_DEMO/img/N200_jobXXXX_task200_best_N200.pdf

Observations and Next Steps

Observed Behavior

- Small N: dense, visually near-optimal packings
- Large N: increasing slack, empty regions near boundary, disordered orientations

Immediate Next Steps

- **Post-processing (cheap):** greedy projection + shrink loop (boundary tightening)
- **Local refinement:** introduce smooth penalties and apply L-BFGS-B
- **Structure discovery:** periodic-boundary SA to find motifs, then tile into near-square patches

Summary

- Non-convex polygon packing solved with **two-phase SA** + robust geometry checks.
- **Area bound** provides provable infeasibility cutoff.
- **Bracket + bisection** yields a tight feasible L reliably.
- **Time-limited polish** improves L under strict HPC budgets and guarantees artifacts.
- Sweep diagnostics quantify **density**, **boundary waste**, and **structural disorder**.

Next steps:

- periodic-boundary runs to estimate infinite-tiling density,
- template/warm-start based on discovered motifs,
- targeted long-polish on hard N values.

Questions?