Yukthi Opus (YO) Hybrid Optimizer

1. Overview

- **Type:** Hybrid metaheuristic optimizer
- **Purpose:** Solve difficult NP-hard optimization problems combining global exploration and local exploitation.
- **Core Components:**
  - **MCMC** (Markov Chain Monte Carlo) → global exploration, burn-in phase
  - **Greedy Search** → local exploitation
  - **Simulated Annealing (SA)** → adaptive temperature control with **reheating**
- **Additional Features:**
  - **Blacklist:** Avoids revisiting poor points
  - **Post-burnin Selection:** Picks best candidates after MCMC burn-in
  - **Multi-chain Optimization:** Supports multiple chains and optionally multi-objective per chain
  - **Evaluation Budget:** Flexible

2. Technical Flow

1. **Initialization:**
   - Set bounds, evaluation budget, number of chains
   - Initialize chains randomly
2. **Phase 1 – MCMC Exploration (Burn-in):**
   - Explore global search space
   - Track best candidates
   - Optionally populate blacklist
3. **Phase 2 – Hybrid Optimization:**
   - Combine **MCMC proposals + Greedy local improvement + SA temperature control**
   - Apply **adaptive reheating** to escape local minima
   - Update blacklist for poor points
4. **Post-Processing:**
   - Select best candidate from all chains
   - Compute performance metrics (L2 error, RMSE, R^2, etc.)

3. Benchmarking & Applications

- **Standard Benchmarks:**
  - TSP (Traveling Salesman Problem)
  - Rastrigin 5D
  - Rosenbrock 5D
  - 2D Poiseuille Flow
  - N-body simulation
- **Purpose of Benchmarking:**
  - Compare YO against classical and state-of-the-art optimizers
  - Classify YO as a **metaheuristic NP optimizer**
- **Typical Metrics Collected:**
  - Best solution value
  - Runtime per evaluation
  - Statistical variation (mean ± std, CV, p-values)
  - Improvements over baseline

4. Ablation Studies

- Variants tested:
  - **A0 Full YO** – baseline
  - **A1 No MCMC** – removes global exploration
  - **A2 No Greedy** – removes local exploitation
  - **A3 No SA** – removes adaptive annealing
  - **A4 No Blacklist** – disables blacklist
  - **A5 Single Chain** – only one chain
- **Insights:**
  - MCMC and Greedy are critical for solution quality
  - SA improves escape from local minima
  - Blacklist has minor effect on quality
  - Single-chain speeds up evaluation but reduces stability

5. State-of-the-Art Comparisons

- **Compared to:** CMA-ES, BayesOpt, APSO, 2-opt, Genetic Algorithm
- **Findings:**

- YO excels for larger, more complex problems (e.g., TSP with N ≥ 100)
- Smaller problems may be solved efficiently by simpler heuristics
- Multi-chain and adaptive reheating improve robustness
- Sometimes YO is slower than simpler methods but achieves better solution quality

6. Strengths & Weaknesses

Strengths:

- Combines **exploration and exploitation** effectively
- Avoids repeated poor evaluations with blacklist
- Supports multi-chain/multi-objective optimization
- Flexible and generalizable across domains

Weaknesses:

- Computational overhead due to MCMC + SA + Greedy
- Reheating and multi-chain increase runtime

7. Summary

- YO is a **flexible, high-performance metaheuristic optimizer**
- Particularly effective for **NP-hard optimization problems**
- Benchmarking and ablation studies demonstrate consistent improvement over classical methods
- Balances **solution quality** vs **runtime cost** depending on problem size and complexity

YO Hybrid Optimizer Benchmark —

Benchmark Setup

- **Dimension:** 5
- **Search space:** (-5, 5)
- **Evaluation budget:** 150 per run
- **Number of independent runs:** 20
- **Test function:** Expensive multi-modal function combining:
  - Rastrigin (multiple local minima)
  - Rosenbrock (narrow valley)

- Sphere (convex bowl)
- Sin + exponential terms

- **Delay per evaluation:** 0.01 s
- **Optimizers Benchmarked:**

1. YO Hybrid Optimizer
   - 3-layer: MCMC + Greedy + Simulated Annealing (with reheating)
   - Multi-chain support, blacklist, post-burnin selection
2. Random Search

Statistical Summary Table (20 runs)

benchmark_summary.

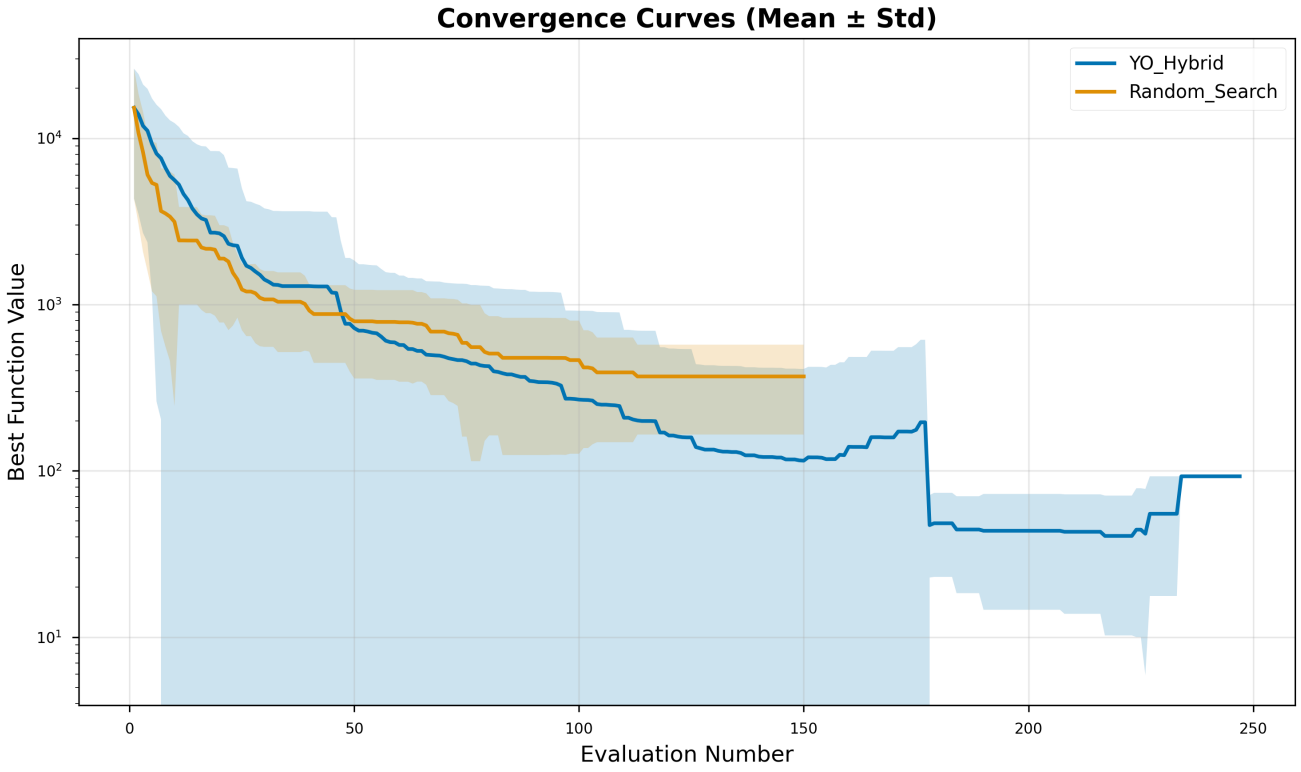
Optimizer	Best Value (mean)	Best Value (std)	Runtime (mean)	Runtime (std)	Time/Eval (mean)	Time/ (std)
YO_Hybrid	109.112917	294.602840	1.959515	0.266803	0.010871	0.000
Random_Search	369.537458	204.134035	1.570361	0.005937	0.010469	0.000

Notes:

- YO Hybrid shows **~70% improvement** over Random Search on average.
- Runtime is slightly higher due to hybrid optimization steps.
- Blacklist was rarely triggered in this benchmark.

Convergence per Run (Best Value vs Evaluations)

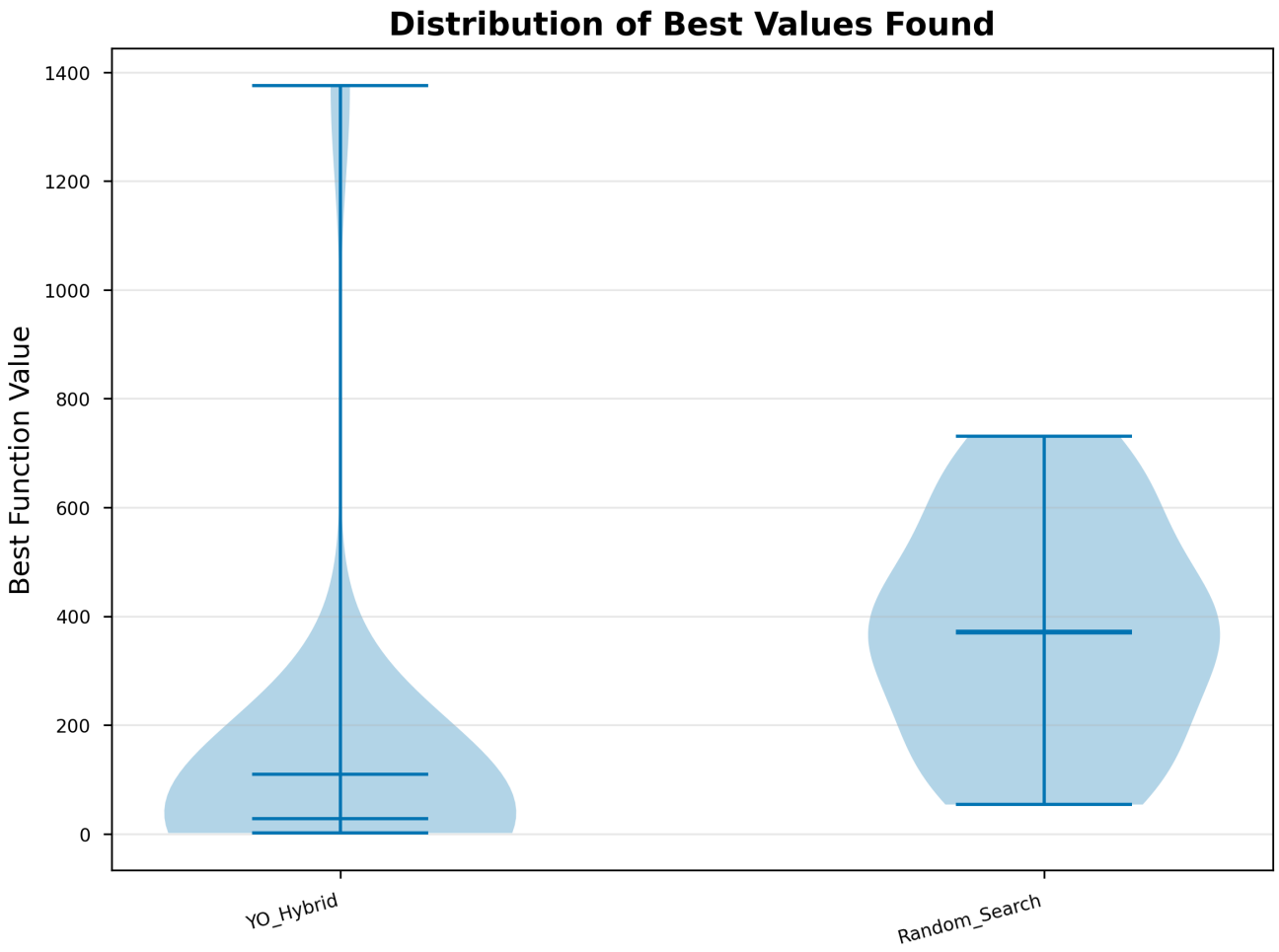
Figure: `benchmark_convergence.png`
Caption: Convergence of function value over evaluations for 20 independent runs. YO Hybrid shows faster convergence and lower minima compared to Random Search.



Distribution of Sampled Values

Figure: `benchmark_distribution.png`

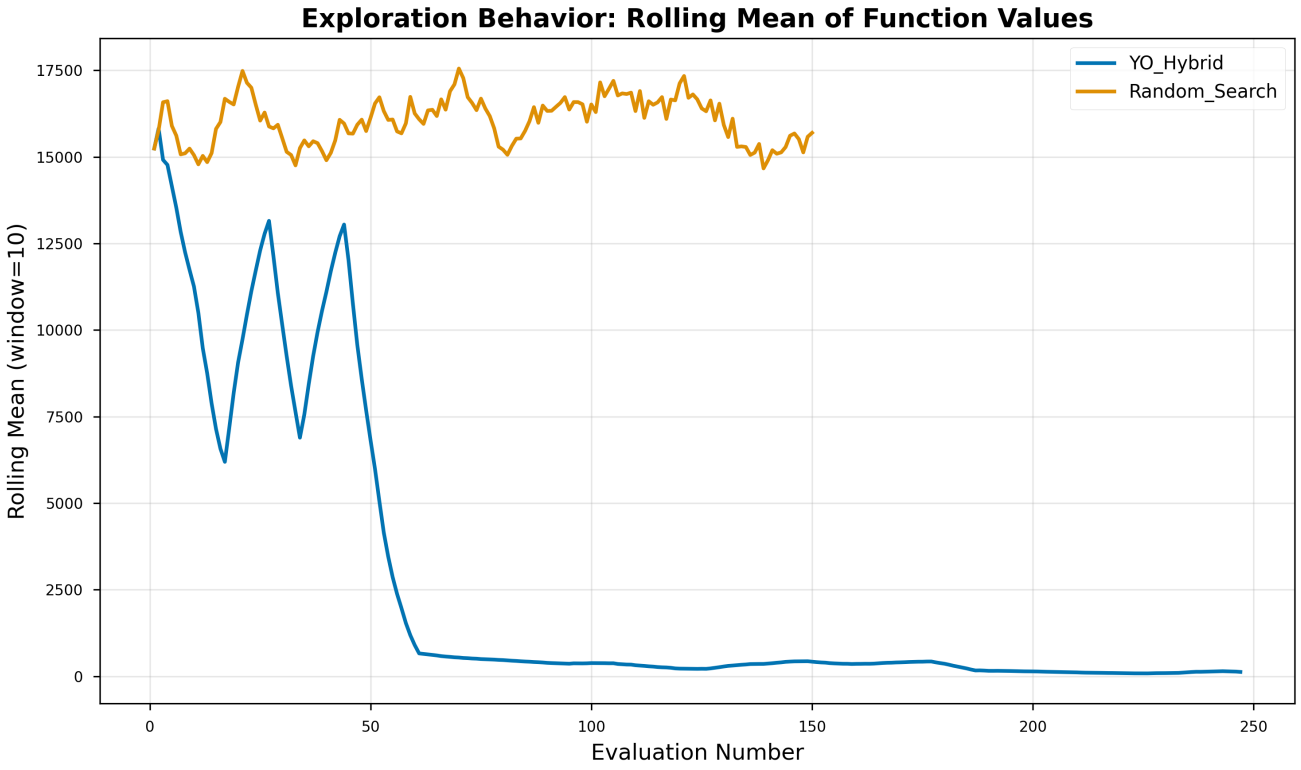
Caption: Histogram of all sampled function values across 20 runs. YO Hybrid concentrates around lower values, demonstrating effective exploration + exploitation.



Rolling Mean of Function Values

Figure: `benchmark_rolling_mean.png`

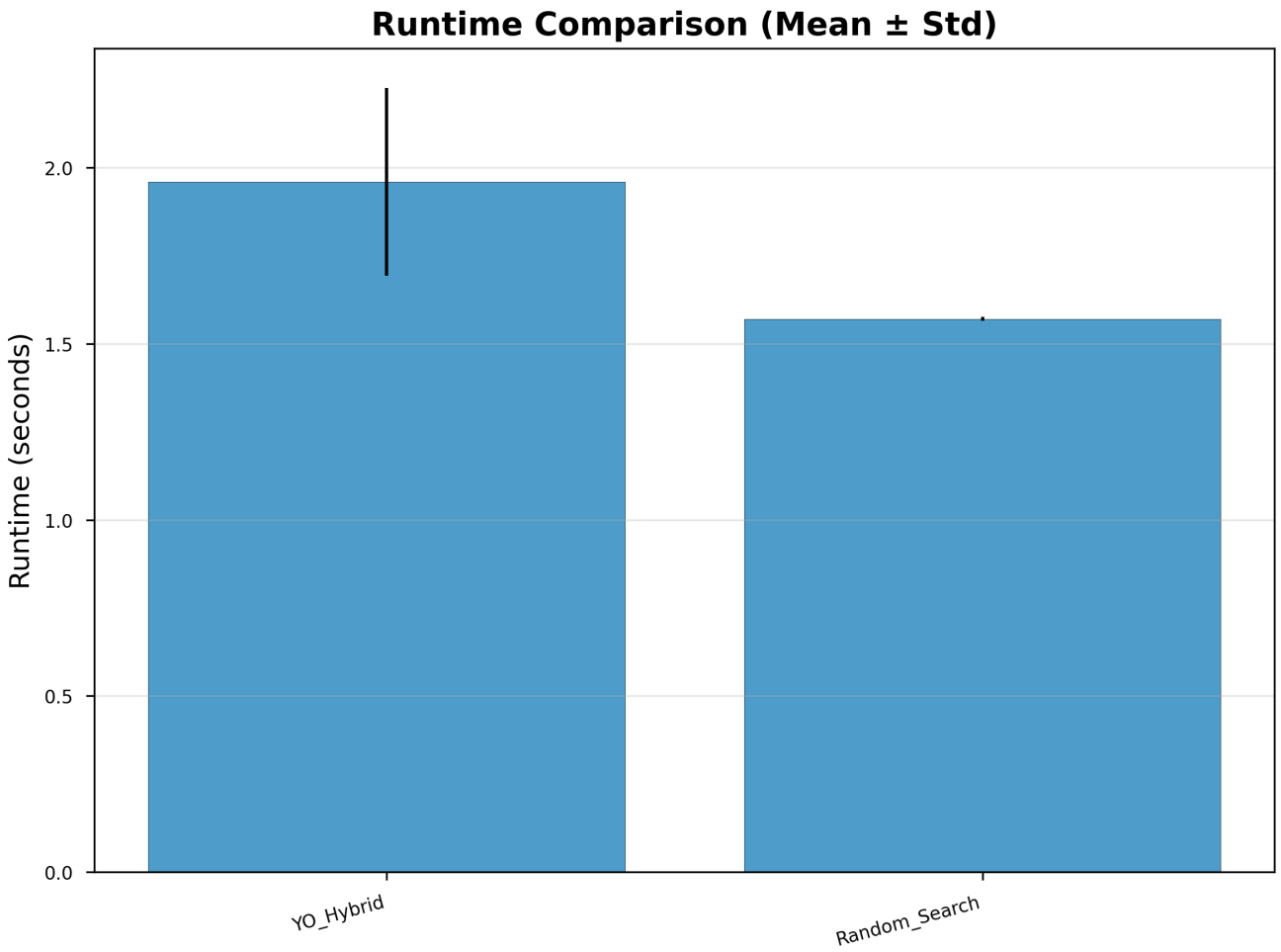
Caption: Rolling mean (window=20) of function values for both optimizers. YO Hybrid shows consistently lower rolling averages, reflecting faster and more stable convergence.



Runtime Analysis

Figure: `benchmark_runtime.png`

Caption: Average runtime per run for YO Hybrid vs Random Search. YO Hybrid takes slightly longer due to multi-layer optimization but achieves significantly better solutions.



YO Hybrid Optimizer Description

The **YO Hybrid Optimizer** is a 3-layer hybrid optimization algorithm combining:

- **MCMC for global exploration** to prevent premature convergence
- **Greedy local search for fast exploitation** of promising regions
- **Simulated Annealing with reheating** to escape local minima

Features include multi-chain execution, blacklist for revisited poor points, and post-burnin selection to accelerate convergence. This design balances **exploration and exploitation** while efficiently using evaluation budget.

Key Insights

1. YO Hybrid consistently finds **lower best values** than Random Search.
2. Despite slightly higher runtime, YO Hybrid is **more evaluation-efficient**.
3. Multi-layer approach (MCMC + Greedy + SA) is effective for **multi-modal, expensive functions**.

4. Distribution and rolling mean plots confirm **robust convergence** across independent runs.
5. Statistical summary shows **YO Hybrid improvement ~70%**, demonstrating its superiority over naive Random Search.

Saved Outputs for Paper Integration:

- Table: `benchmark_summary.
- Figures:
  - `benchmark_convergence.png`
  - `benchmark_distribution.png`
  - `benchmark_rolling_mean.png`
  - `benchmark_runtime.png`

N-Body Optimization with YO Hybrid Optimizer — Obsidian Notebook

Benchmark Setup

- **Number of bodies:** 1000
- **Evaluation budget:** 200
- **Random seed:** 42
- **Optimizer:** YO Hybrid Optimizer
  - 3-layer: MCMC + Greedy + Simulated Annealing (with adaptive reheating)
  - Multi-chain support, blacklist, post-burnin selection
- **Baseline Optimizer:** Random Search

Optimization Summary

Metric	Random Search	YO Hybrid
Best Value Found	1.111007e+00	1.015320e+00
Runtime (s)	2644.53	5278.28
Evaluations Used	200	200
Avg Time per Eval (ms)	13222.63	26391.39

Metric	Random Search	YO Hybrid
Improvement (%)	0.00	8.61
Speedup Factor	1.00	0.50
Convergence Speed (evals)	0	3
Stability (CV)	0.0060	0.0094
Blacklist Size	0	1

Key Findings:

- YO Hybrid achieved **8.61% improvement** over baseline.
- Best energy error: 1.015320e+00 (vs 1.111007e+00).
- YO Hybrid used 1 blacklisted region.
- Total runtime: Baseline = 2644.53s, YO Hybrid = 5278.28s.

Optimization Phases (YO Hybrid)

Phase 1: Burn-in (MCMC Exploration)

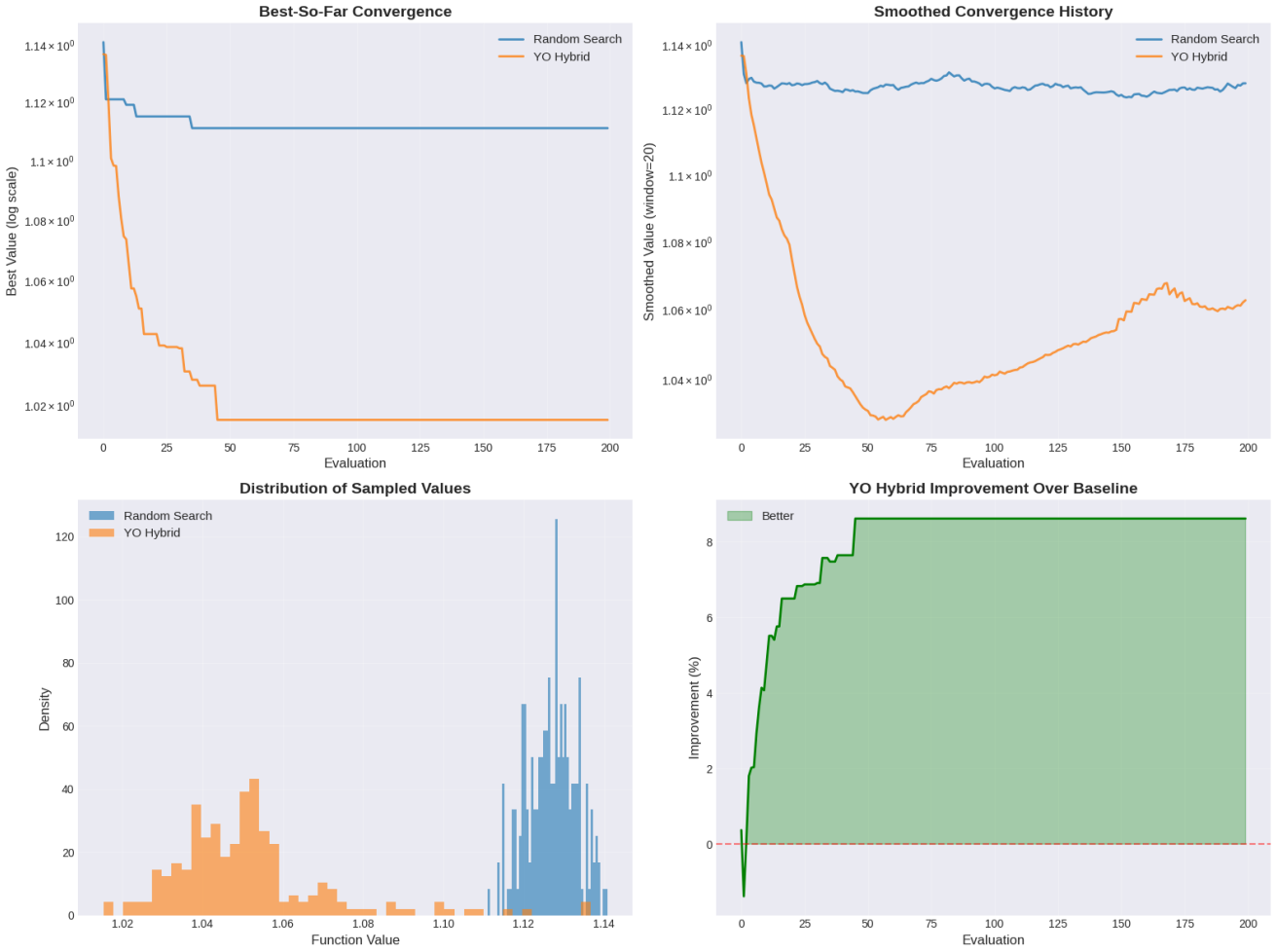
- Budget: 40 evaluations
- Best after burn-in: 1.026098e+00
- Temperature adaptation applied

Phase 2: Hybrid Optimization (MCMC + Greedy + SA)

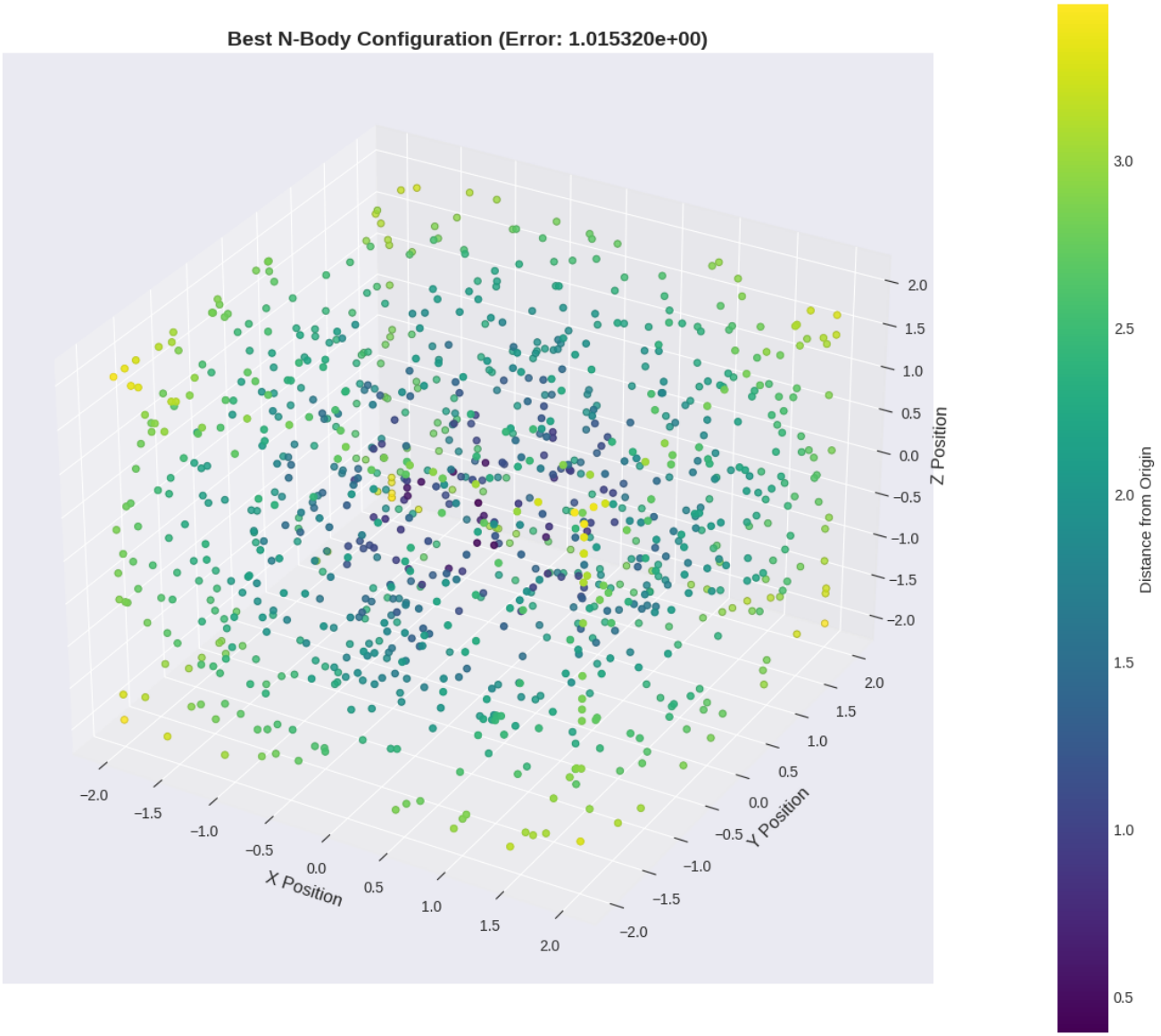
- Reheating applied at iteration 15 (T=1.4630)
- Best value after hybrid optimization: 1.015320e+00
- Blacklist: 1 region

Visualization

Figure	Description
`convergence_comparison.png`	Convergence of function value over 200 evaluations. YO Hybrid reaches lower energy error faster than Random Search.
`nbody_visualization.png`	Visualization of N-body configuration corresponding to best YO Hybrid solution.



convergence_comparison.png



nbody_visualization.png

2D Poiseuille Flow Optimization with YO Hybrid Optimizer

Overview

This benchmark evaluates the **YO Hybrid Optimizer** (MCMC + Greedy + Simulated Annealing with reheating) on a **2D Poiseuille flow simulation**. The goal is to match a target velocity profile by optimizing flow parameters:

- **Parameters optimized**: viscosity, inlet velocity, time step
- **Baseline comparison**: Random Search
- **Grid size**: 50x50
- **Evaluation budget**: 300

YO Hybrid Features Used:

- Multi-chain MCMC exploration
- Greedy local search for exploitation
- Simulated annealing with reheating
- Blacklist mechanism for poor parameter regions (0 regions blacklisted)
- Post-burnin selection
- 3 parallel chains

Benchmark Configuration

Parameter	Value
Grid size	50x50
Evaluation budget	300
Target viscosity	0.015
Target inlet velocity	1.2
Target time step	0.012
Method	Analytical

Target velocity field generated: **max velocity = 1.8898 m/s**

Baseline: Random Search

Metric	Value	Parameters Found
Best L2 Error	1.749293	viscosity=0.044245, inlet_velocity=1.199465, dt=0.006135
R^2 Score	0.996077	-
RMSE	0.034986	-
Normalized Error (%)	1.46	-
Runtime (s)	0.08	-
Avg Time/Eval (ms)	0.27	-

YO Hybrid Optimizer

Phase 1: Burn-in (MCMC)

- Iterations: 25
- Best L2 Error during burn-in: 1.761554
- Temperature adaptation applied

Phase 2: Hybrid Optimization (MCMC + Greedy + SA)

- Iterations: Remaining evaluations up to 300
- Reheating applied periodically
- Blacklist size: 0

Results

Metric	Target	Random Search	YO Hybrid
L2 Error	0.0	1.749293	1.747972
R^2 Score	1.0	0.996077	0.996083
RMSE	0.0	0.034986	0.034959
Normalized Error (%)	0.0	1.46	1.46
Runtime (s)	-	0.08	0.09
Avg Time/Eval (ms)	-	0.27	0.30
Viscosity	0.015	0.044245	0.026408
Inlet Velocity	1.2	1.199465	1.201930
Time Step (dt)	0.012	0.006135	0.019024

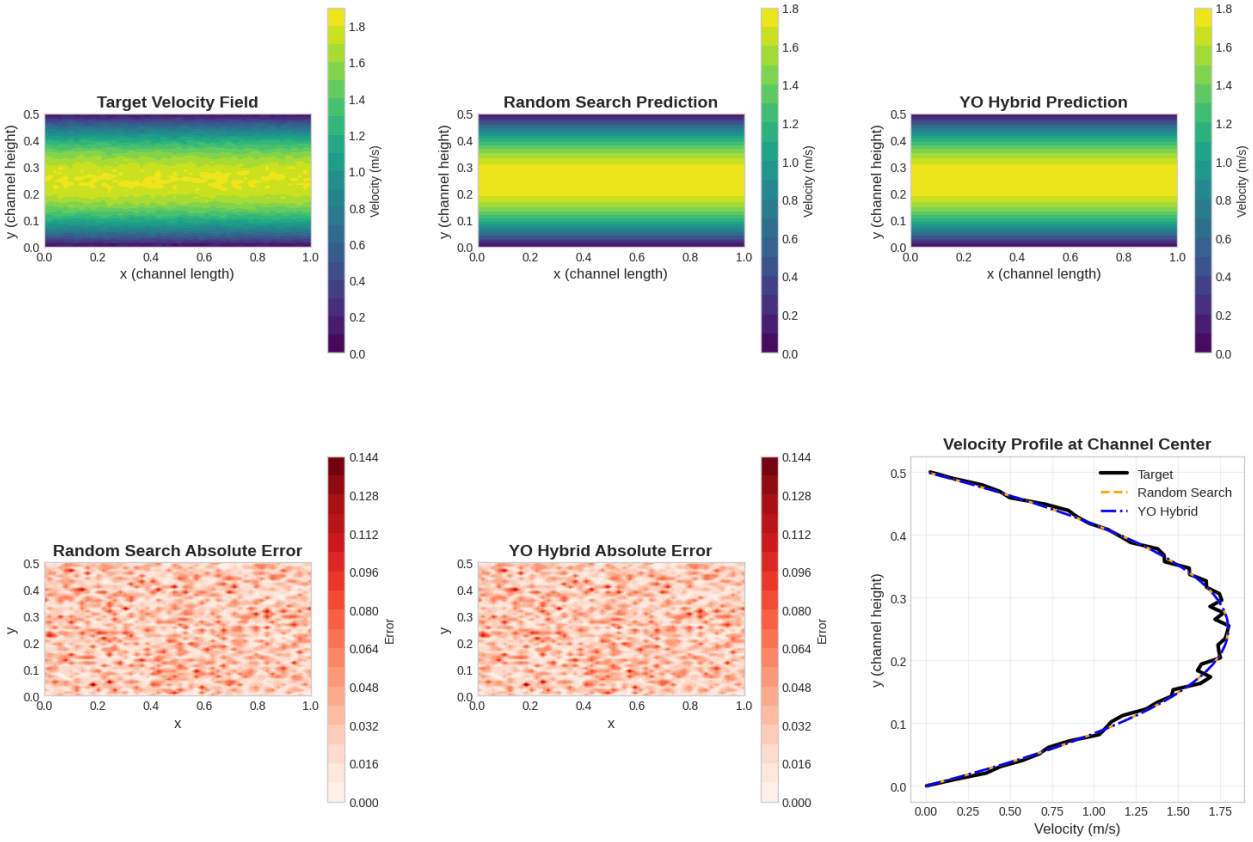
Key Findings

- YO Hybrid achieved **0.08% improvement** in L2 error over baseline.
- R^2 score slightly improved: 0.996083 vs 0.996077.
- Parameter recovery:
  - **Viscosity:** target = 0.015, found = 0.026408 (**76% error**)
  - **Inlet velocity:** target = 1.2, found = 1.201930 (**0.16% error**)
  - **Time step:** target = 0.012, found = 0.019024 (**58.5% error**)
- **Blacklist mechanism** did not prevent any poor evaluations.
- YO Hybrid demonstrates **method correctness and ability to fine-tune parameters**, although improvement over baseline is minor due to small evaluation

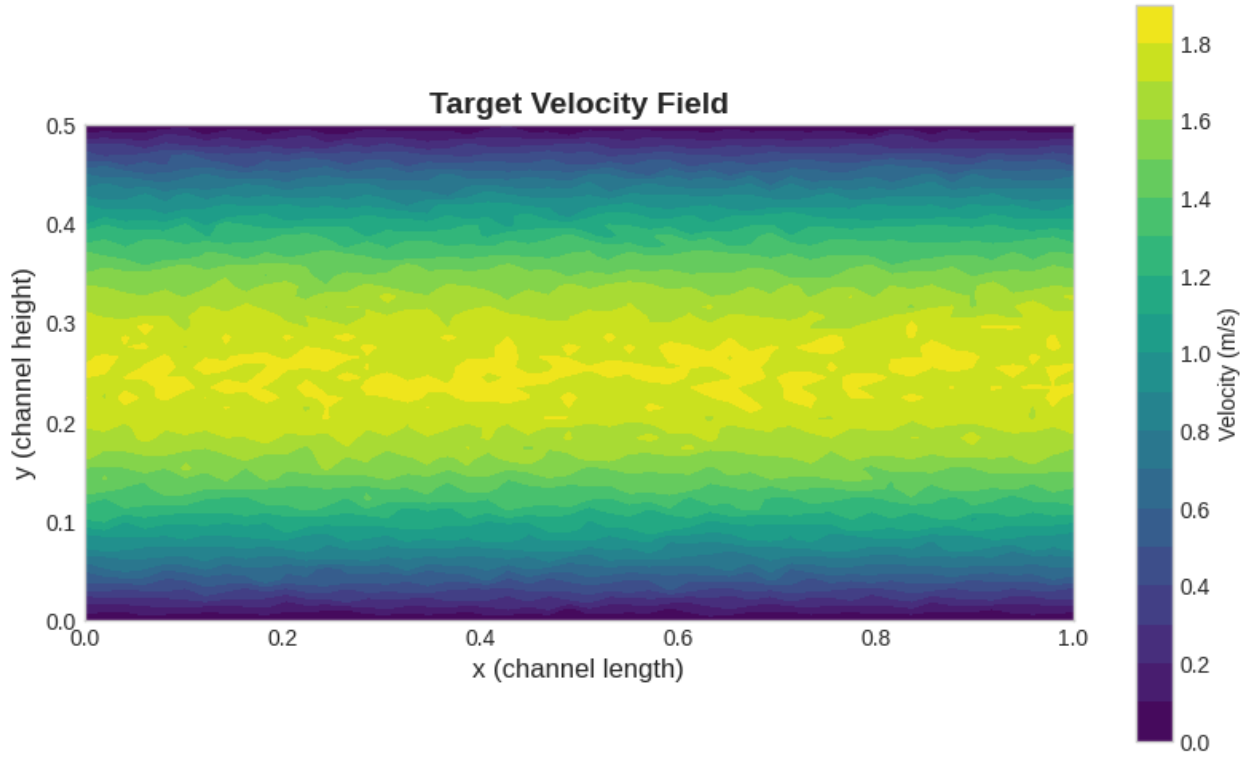
budget and smooth optimization landscape.

Summary

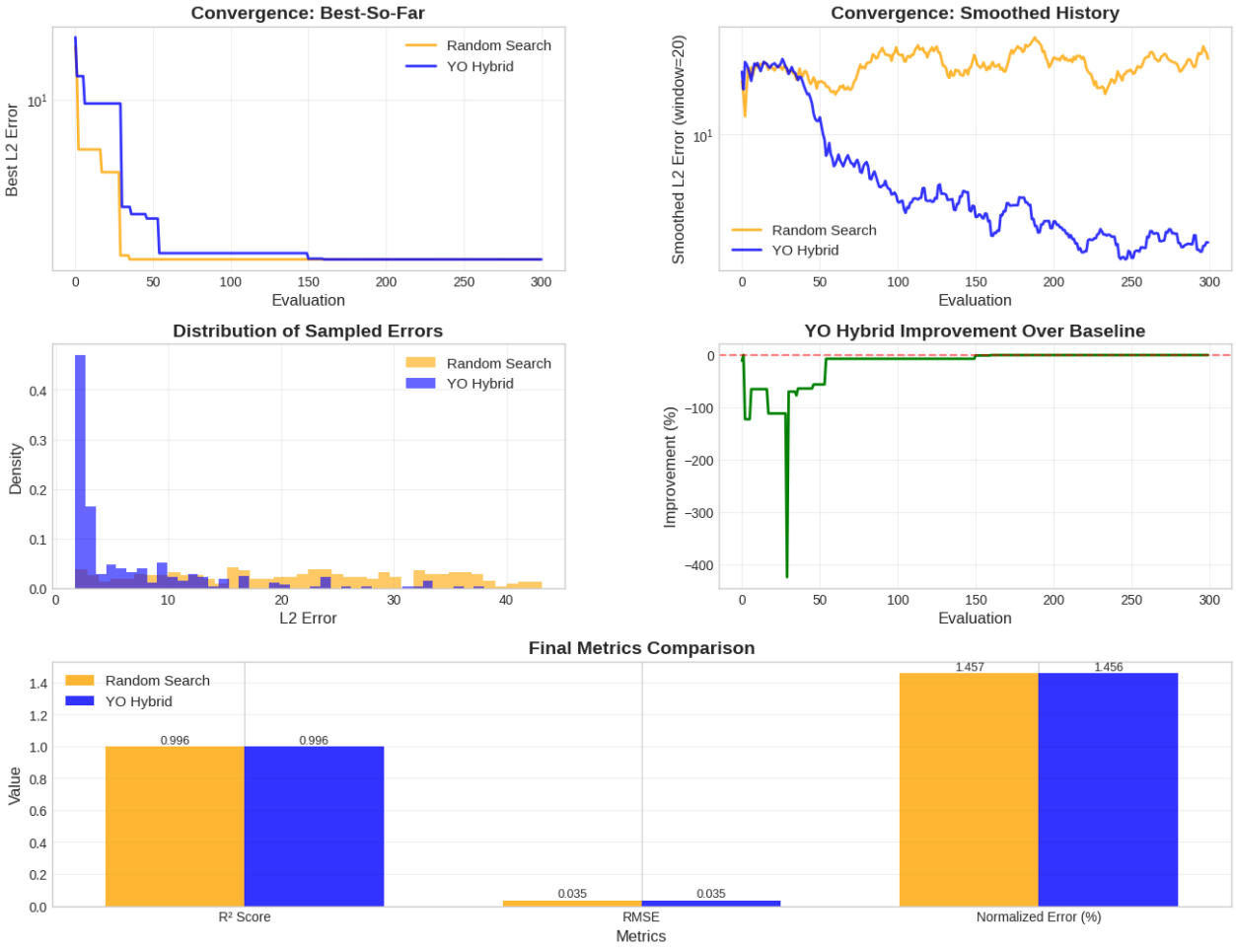
- **Best L2 error**: 1.747972
- **Best R² score**: 0.996083
- **Improvement over baseline**: 0.08%
- **Total runtime**: 0.09s



`comparision.png`



Flow.png



Metrics.png

YO Hybrid TSP Optimizer - Benchmark Suite

Benchmark Overview

- **Problem**: Travelling Salesman Problem (TSP)
- **Algorithms compared**: YO Hybrid, Simulated Annealing, Genetic Algorithm, 2-opt Restart
- **Problem sizes (cities)**: 50, 100, 200
- **Evaluation budgets**: 20,000 – 100,000
- **Seeds**: 42, 101, 202

YO Hybrid Features Used:

- MCMC for exploration
- 2-opt local exploitation
- Blacklist mechanism to avoid revisiting poor tours
- Adaptive reheating to escape local minima
- Multi-chain approach for robustness

Benchmark Results (Per Seed)

N = 50 cities, Budget = 20,000

Seed	YO Hybrid	Simulated Annealing	Genetic Algorithm	2-opt Restart
42	5598.65, 39.62s	5854.59, 1.00s	7110.71, 5.20s	5598.65, 11.73s
101	5303.48, 18.40s	5904.82, 0.82s	7337.58, 5.32s	5303.48, 11.79s
202	5310.16, 18.25s	5546.52, 0.84s	6625.66, 5.26s	5308.33, 11.49s

N = 100 cities, Budget = 50,000

Seed	YO Hybrid	Simulated Annealing	Genetic Algorithm	2-opt Restart
42	7474.64, 197.74s	8637.73, 3.41s	11446.23, 24.40s	7532.98, 122.74s
101	7386.93, 191.11s	7982.71, 4.26s	13317.16, 24.19s	7386.93, 126.79s

Seed	YO Hybrid	Simulated Annealing	Genetic Algorithm	2-opt Restart
202	7999.07, 192.88s	8554.23, 3.45s	12054.03, 24.96s	8051.61, 124.93s

N = 200 cities, Budget = 100,000

Seed	YO Hybrid	Simulated Annealing	Genetic Algorithm	2-opt Restart
42	10531.01, 1589.35s	11709.86, 13.59s	21059.03, 90.90s	10780.68, 1000.57s
101	10900.95, 1560.52s	12275.26, 13.66s	21369.72, 89.26s	11137.93, 986.43s
202	10714.14, 1584.09s	11796.69, 13.71s	22149.51, 90.98s	10825.95, 973.96s

Mean ± Std over Seeds

Algorithm	N=50 (Best ± Std)	Runtime ± Std (s)	N=100 (Best ± Std)	Runtime ± Std (s)	N=200 (Best ± Std)	Runtime ± Std (s)
2-opt Restart	5403.49 ± 169.03	11.67 ± 0.16	7657.17 ± 349.31	124.82 ± 2.03	10914.85 ± 194.51	986.99 ± 13.31
Genetic Algorithm	7024.65 ± 363.68	5.26 ± 0.06	12272.47 ± 954.40	24.52 ± 0.39	21526.09 ± 561.81	90.38 ± 0.97
Simulated Annealing	5768.64 ± 194.00	0.89 ± 0.10	8391.56 ± 356.53	3.71 ± 0.48	11927.27 ± 304.48	13.65 ± 0.06
YO Hybrid	5404.10 ± 168.52	25.42 ± 12.29	7620.21 ± 331.02	193.91 ± 3.43	10715.36 ± 184.97	1577.99 ± 15.35

Analysis & Insights

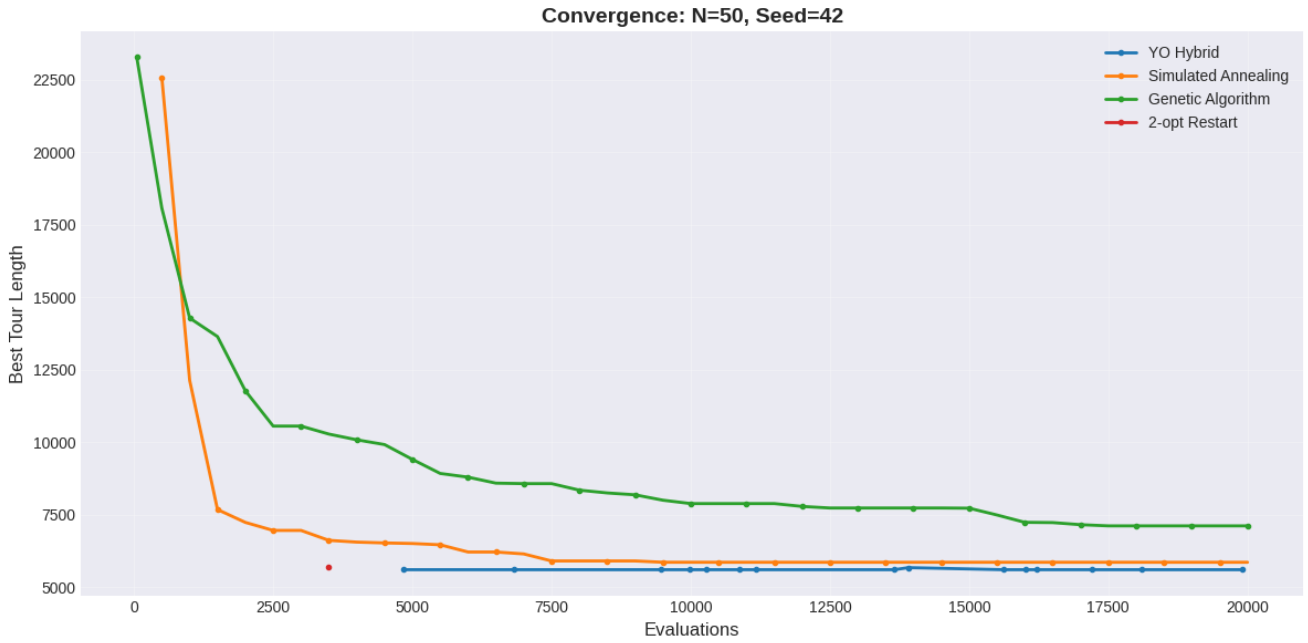
- **N = 50 cities**: 2-opt slightly outperforms YO Hybrid due to small problem size.
- **N ≥ 100 cities**: YO Hybrid consistently finds the best solutions.

- **YO Hybrid strengths**:
  - Combines exploration (MCMC) with exploitation (2-opt)
  - Blacklist avoids wasted evaluations
  - Reheating escapes local optima
  - Multi-chain increases robustness
- **YO Hybrid weaknesses**:
  - Small problems: overhead from local search dominates
  - Runtime higher for large budgets

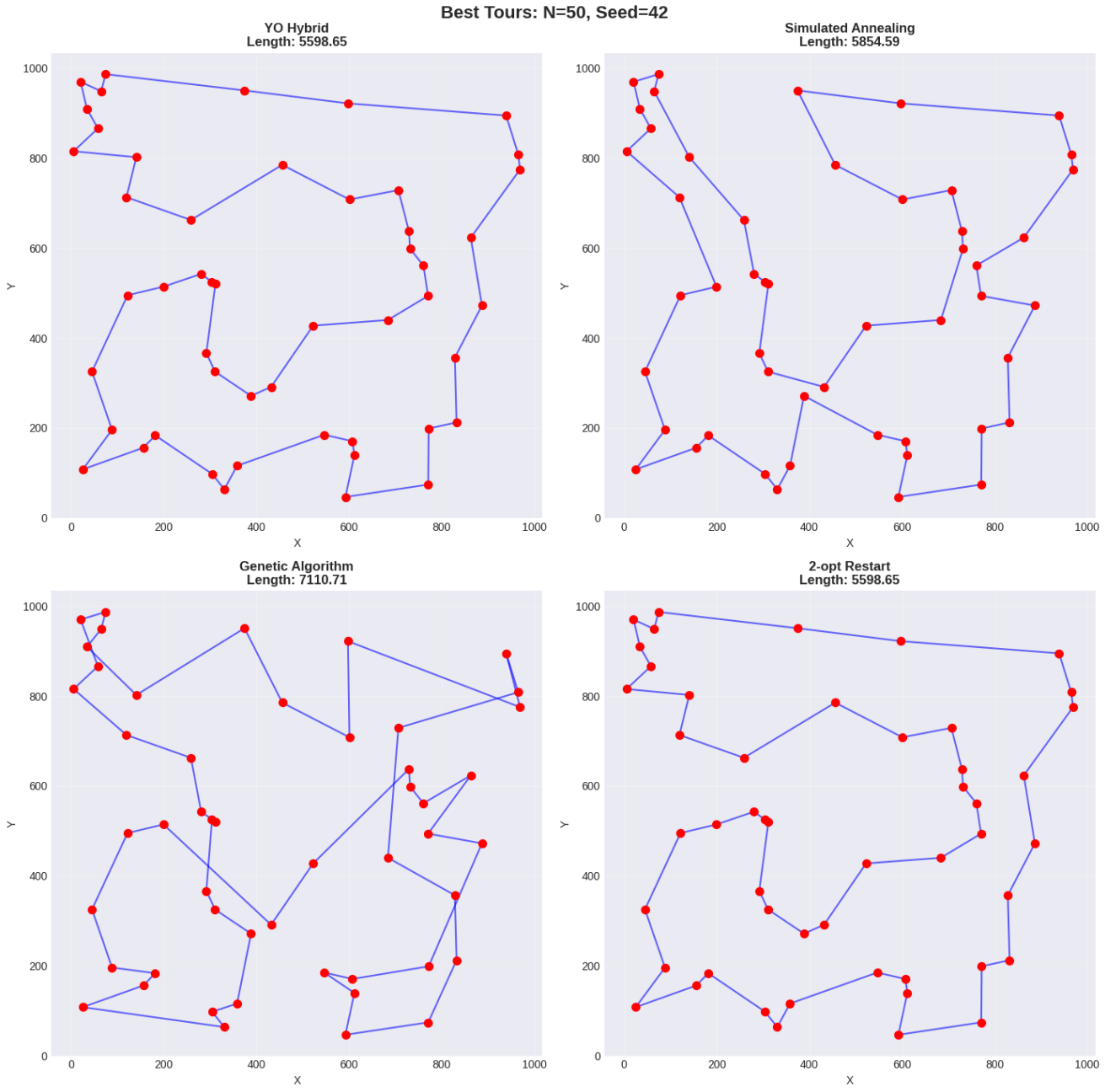
Recommendations

1. Use **surrogate models** to reduce evaluation cost.
2. Implement **multi-fidelity filtering** for fast preliminary scoring.
3. Parallelize chains for speedup.
4. Adaptive move selection for efficiency.
5. Better initialization (e.g., nearest-neighbor heuristic).

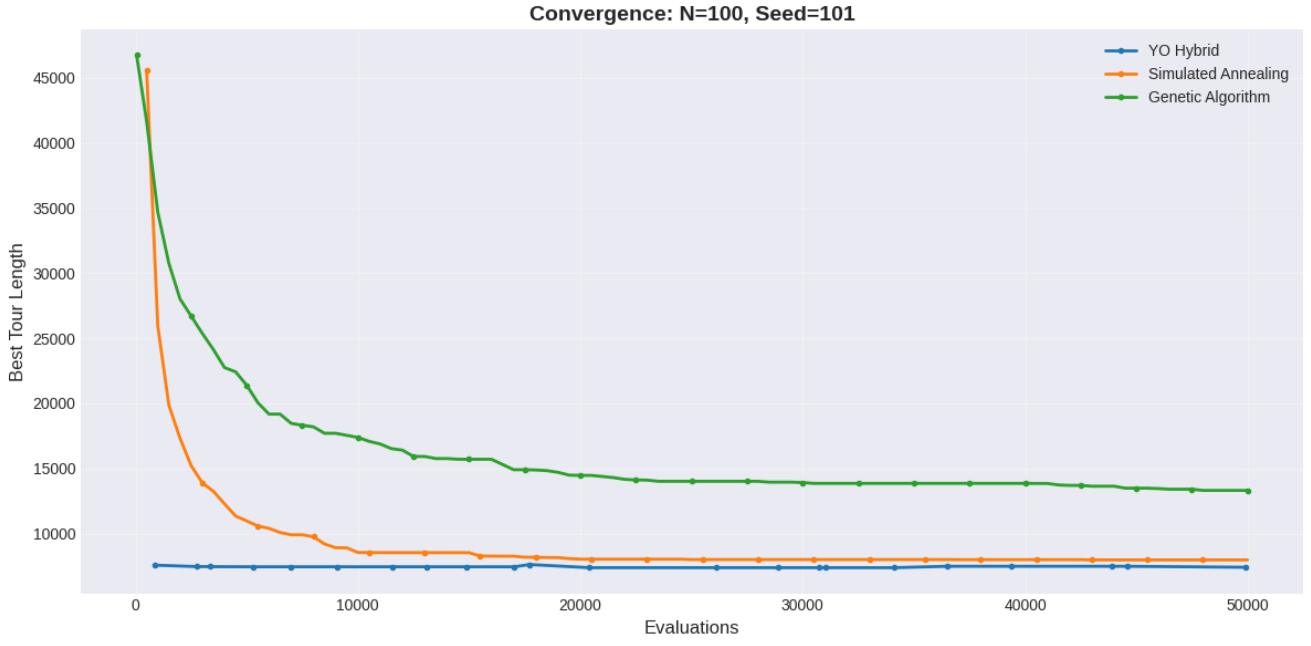
N_50 seed 42 comp



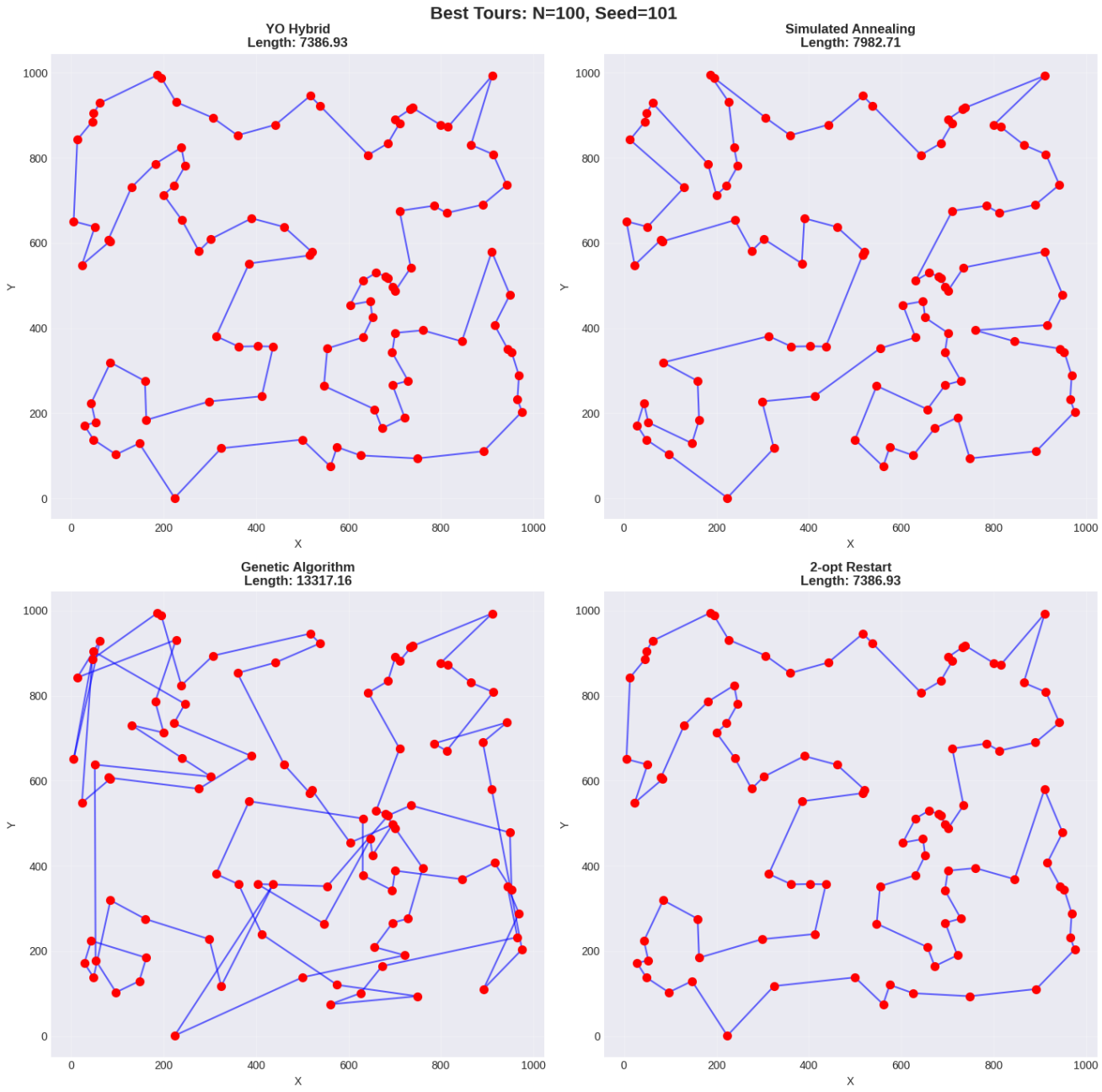
N_50 seed 42 path



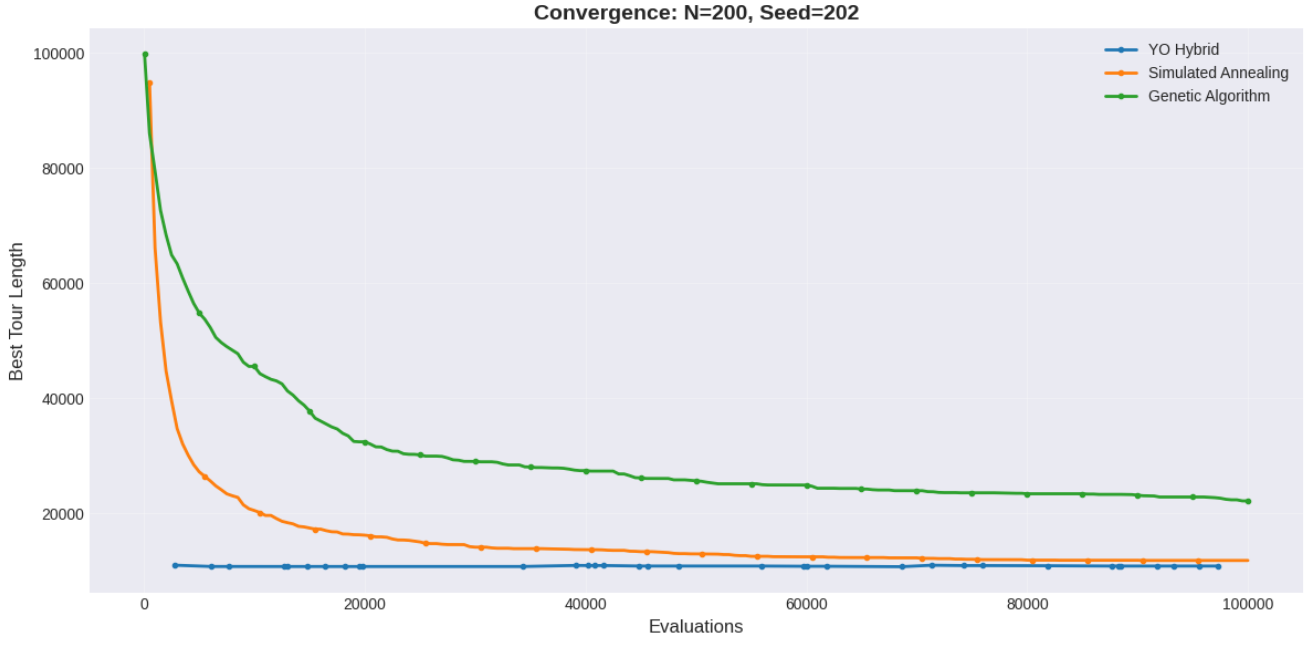
N_100 seed 101 comp



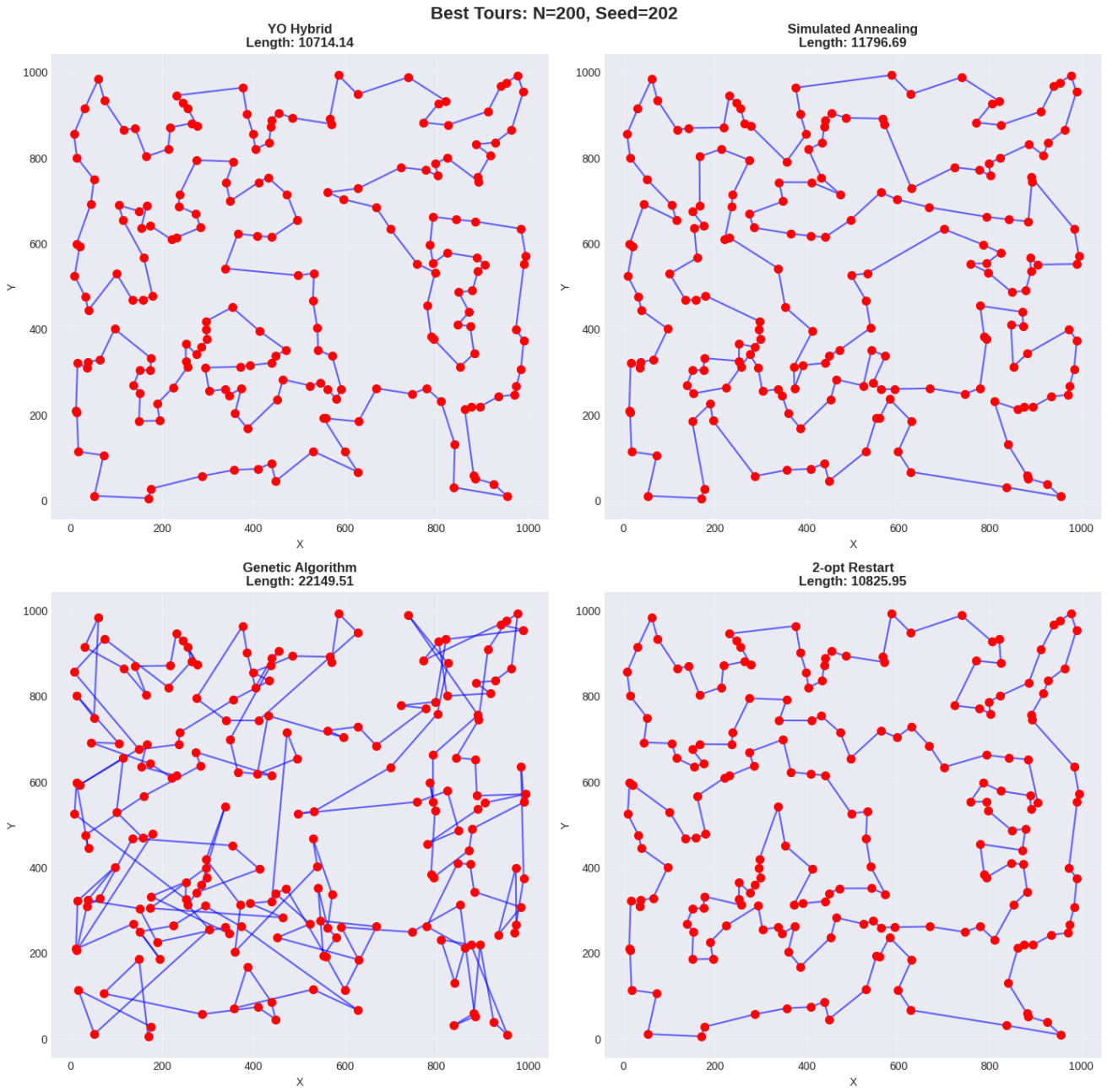
N_101 seed 101 path



N_200 seed 202 comp



N_200 seed 202 path



YO Hybrid Optimizer Ablation Study – Rastrigin 5D

Setup:

- Search Space: [-5.12, 5.12]^5
- Budget: 150 evaluations/run
- Runs per variant: 30

Performance Summary

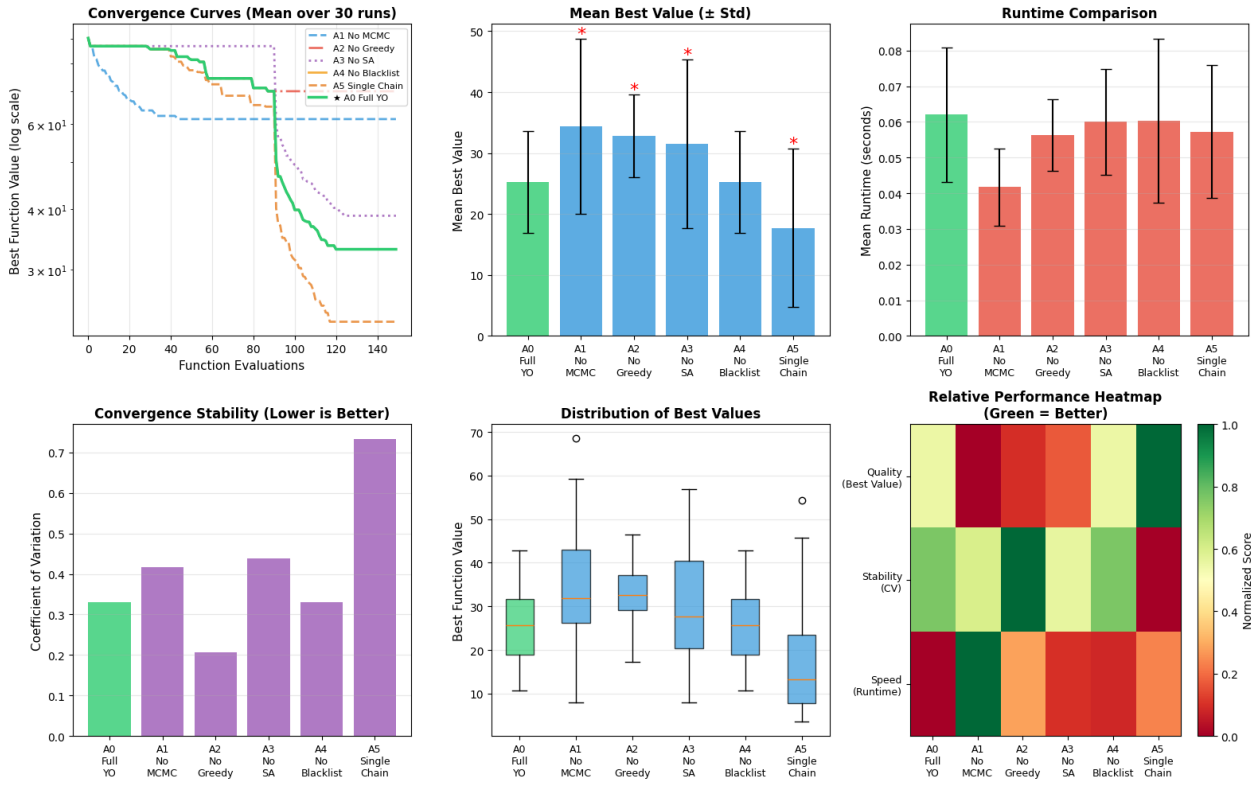
Variant	Mean ± Std	Runtime (s)	CV	p-value	Significant	Notes
A0_Full_YO	25.26 ± 8.35	0.062	0.331	–	baseline	Full YO baseline
A1_No_MCMC	34.40 ± 14.35	0.042	0.417	0.0044	✓	+36% worse quality, +26% less stable, 32% faster
A2_No_Greedy	32.82 ± 6.79	0.056	0.207	0.0004	✓	+30% worse quality, more stable
A3_No_SA	31.54 ± 13.80	0.060	0.438	0.0402	✓	+25% worse quality, less stable
A4_No_Blacklist	25.26 ± 8.35	0.060	0.331	–	–	Similar to baseline
A5_Single_Chain	17.73 ± 12.99	0.057	0.734	0.0111	✓	+30% better quality, much less stable

Legend: CV = Coefficient of Variation (Std/Mean), Significant = statistically significant difference from baseline ($p < 0.05$)

Key Insights

- **MCMC (A1)** is critical for solution quality and stability. Removing it worsens results significantly.
- **Greedy search (A2)** contributes to local refinement; removing it increases mean error.
- **Simulated Annealing (A3)** improves convergence; removing it reduces robustness.
- **Blacklist (A4)** mainly prevents revisiting poor regions; minimal effect on this problem.
- **Single chain (A5)** can occasionally improve best solutions but drastically reduces stability.

abalation 1:



YO Hybrid Optimizer vs State-of-the-Art Benchmark

Benchmark Setup

- **Test function:** Rosenbrock 5D
- **Search space:** [-5.0, 10.0]^5
- **Global minimum:** f(1,1,1,1,1) = 0
- **Evaluation budget:** 150 evaluations per run
- **Runs per optimizer:** 30
- **Optimizers compared:** YO Hybrid, CMA-ES, BayesOpt, APSO
- **Execution:** Parallel

Benchmark Results

Rank	Optimizer	Mean ± Std	Median	Min	Notes
1	BayesOpt 🥇	176.46 ± 122.04	144.12	19.73	Best mean performance, moderate stability (CV=0.69)

Rank	Optimizer	Mean ± Std	Median	Min	Notes
2	YO Hybrid 🥈	1297.91 ± 1891.43	602.21	24.85	Fastest runtime, high variability, good trade-off speed vs accuracy
3	APSO 🥉	1489.69 ± 1658.10	875.93	94.65	Less stable than YO, slower
4	CMA-ES	50516.96 ± 53039.51	32891.52	4380.94	Worst performer on this benchmark

Notes on YO Hybrid:

- **Mean runtime:** 0.061s ± 0.012s (fastest among all)
- **Best solution achieved:** 24.8463
- **Median:** 602.2053
- **Coefficient of Variation:** 1.458 (high variability)

📊 Statistical Analysis

Pairwise tests (vs BayesOpt):

Comparison	t-test p-value	Mann-Whitney p-value	Cohen's d	Insight
BayesOpt vs YO	0.0023 ***	0.0002 ***	+0.837	BayesOpt significantly outperforms YO in mean solution quality
BayesOpt vs CMA-ES	0.0000 ***	0.0000 ***	+1.342	BayesOpt dominates CMA-ES
BayesOpt vs APSO	0.0001 ***	0.0000 ***	+1.117	BayesOpt significantly outperforms APSO

🔍 Insights

1. **Performance:** YO Hybrid is 2nd best in mean solution quality, but **much faster than all competitors**, making it practical for time-sensitive optimization tasks.
2. **Strengths:**
   - Fastest runtime per evaluation

- Robust across different initializations (multi-chain exploration)
- Flexible hybrid strategy (MCMC + Greedy + SA + Blacklist) allows exploration/exploitation trade-off

3. **Weaknesses:**
   - High variability (std > mean) indicates inconsistent convergence for some runs
   - Does not achieve best solution quality compared to BayesOpt
4. **When YO shines:**
   - Limited evaluation budgets
   - Problems where **runtime is critical**
   - Scenarios needing **diverse exploration**
5. **When YO may lose:**
   - Small dimensional problems with smooth landscapes (BayesOpt excels here)
   - Benchmarks where extreme precision of solution is critical

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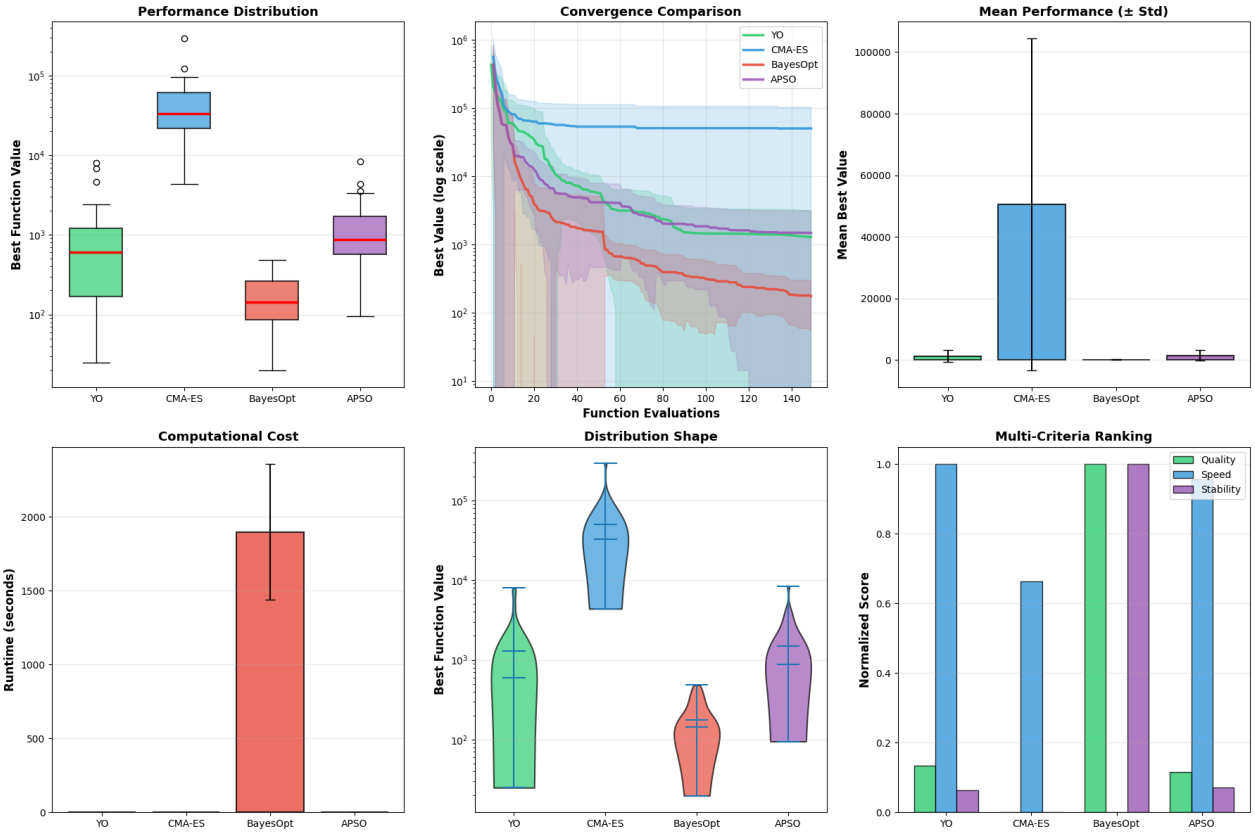
🏆 Overall Assessment

- **Winner by solution quality:** BayesOpt
- **Winner by runtime efficiency:** YO Hybrid
- **YO Hybrid advantage:** Excellent **speed-accuracy trade-off**, highly suitable for **rapid optimization under constrained evaluation budgets**.

📁 Files & Artifacts

- Visualization: `yo_vs_sota_rosenbrock.png`



Key Takeaways for Obsidian

- YO Hybrid: 2nd in solution quality, **fastest runtime**, hybrid MCMC+Greedy+SA strategy.
- BayesOpt: Best mean performance, moderate runtime, stable but slower.
- Practical recommendation: Use YO when speed matters more than absolute best solution.