Modeling Non-Determinism in HPC Applications

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Non-Determinism and Correctness in HPC

- **HPC Community Position:** "Non-determinism control" and "anomaly detection" identified in DOE report on the 2017 HPC Correctness Summit as key challenges in bug detection and localization [1]

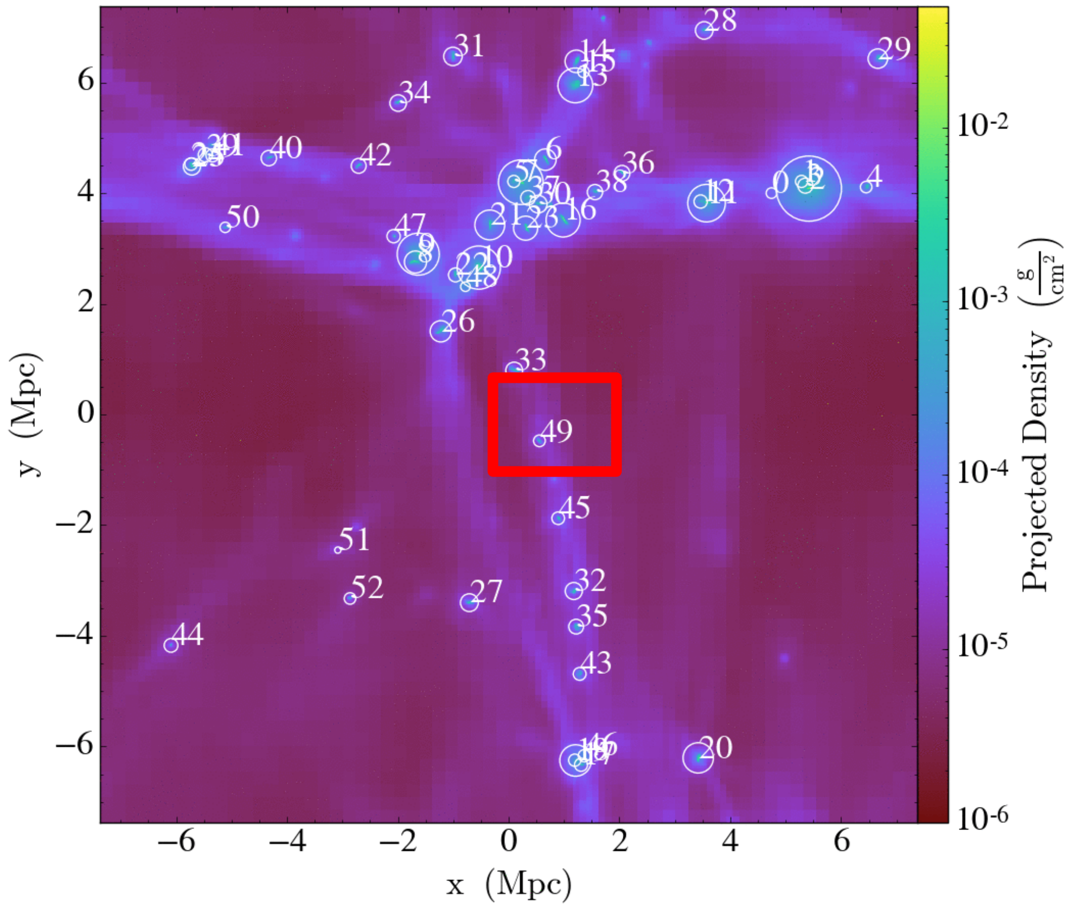
1. Gopalakrishnan, G., Hovland, P.D., Iancu, C., Krishnamoorthy, S., Laguna, I., Lethin, R.A., Sen, K., Siegel, S.F. and Solar-Lezama, A., 2017. Report of the HPC Correctness Summit, Jan 25--26, 2017, Washington, DC. *arXiv preprint arXiv:1705.07478*. See section 3.2.4, 3.2.5

Non-Determinism and Correctness in HPC

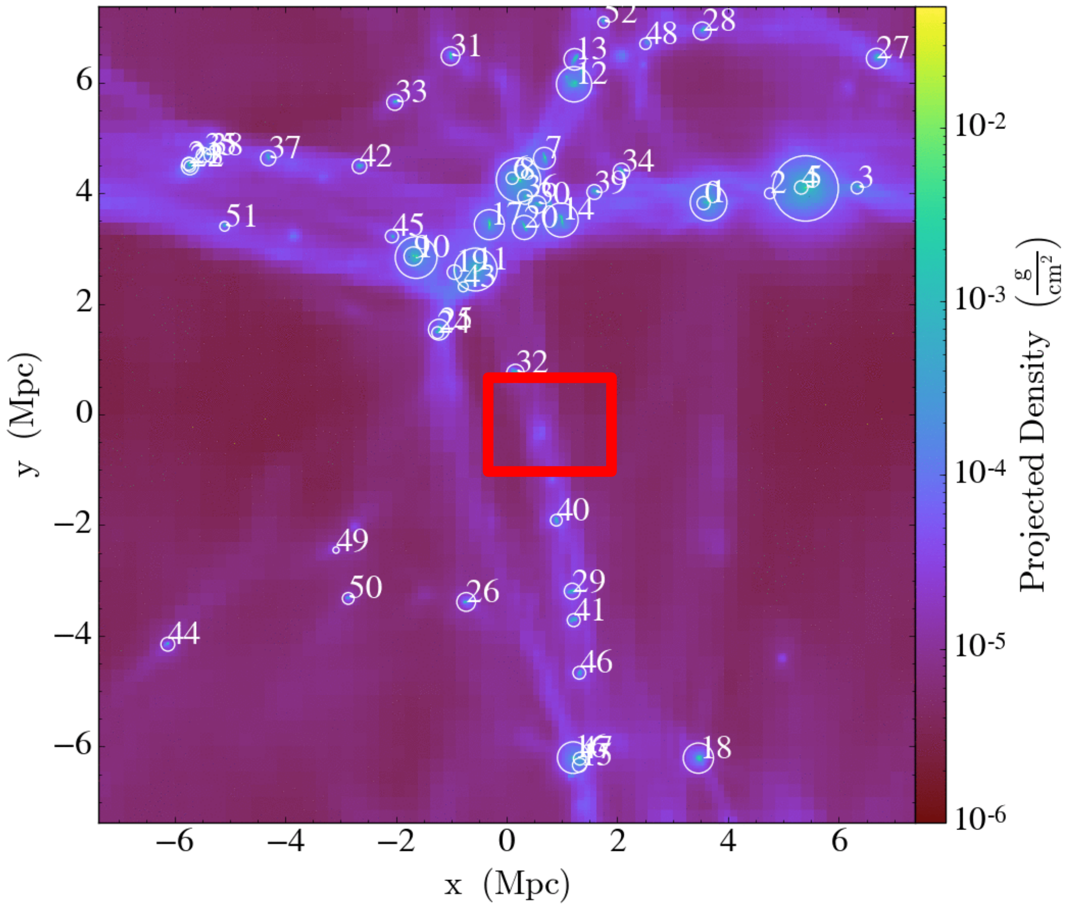
- **HPC Community Position:** "Non-determinism control" and "anomaly detection" identified in DOE report on the 2017 HPC Correctness Summit as key challenges in bug detection and localization [1]
- **Our Position:**
  - These challenges go hand-in-hand.
  - Detecting when and how applications act non-deterministically **in anomalous ways** is critical

1. Gopalakrishnan, G., Hovland, P.D., Iancu, C., Krishnamoorthy, S., Laguna, I., Lethin, R.A., Sen, K., Siegel, S.F. and Solar-Lezama, A., 2017. Report of the HPC Correctness Summit, Jan 25--26, 2017, Washington, DC. *arXiv preprint arXiv:1705.07478*. See section 3.2.4, 3.2.5

Impacts of Non-Determinism on Scientific Outcomes



Run where galactic halo **was detected**



Run where galactic halo was **not detected**

1. Stodden, V. and Krafczyk, M.S., 2018. Assessing Reproducibility: An Astrophysical Example of Computational Uncertainty in the HPC Context.

Interaction Between Non-Associativity and Non-Determinism

$a = 10^9,\ b = -10^9,\ c = 10^{-9}$

Summation order 1

$(a + b) + c = (10^9 - 10^9) + 10^{-9} = 10^{-9}$

Summation order 2

$a + (b + c) = 10^9 + (-10^9 + 10^{-9}) = 0$

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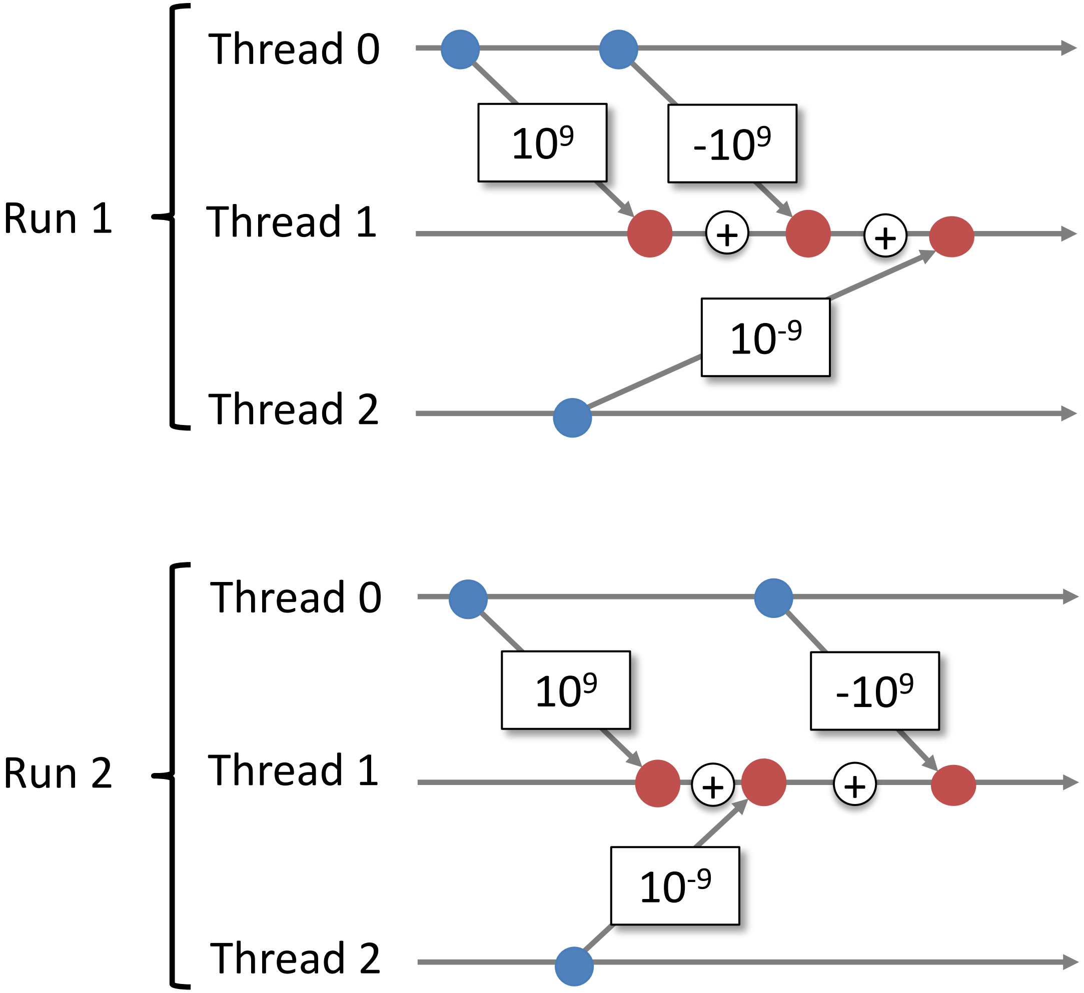
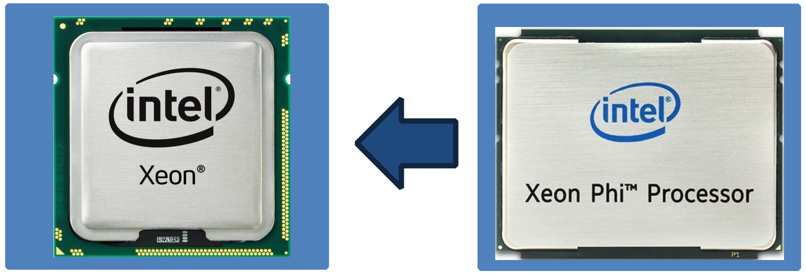


Impacts of Non-Determinism on Correctness

Example 1:

- Rounding difference between Xeon CPU and Xeon Phi caused message count to differ on CPU code vs. accelerator code [1]
- Message count difference induced deadlock

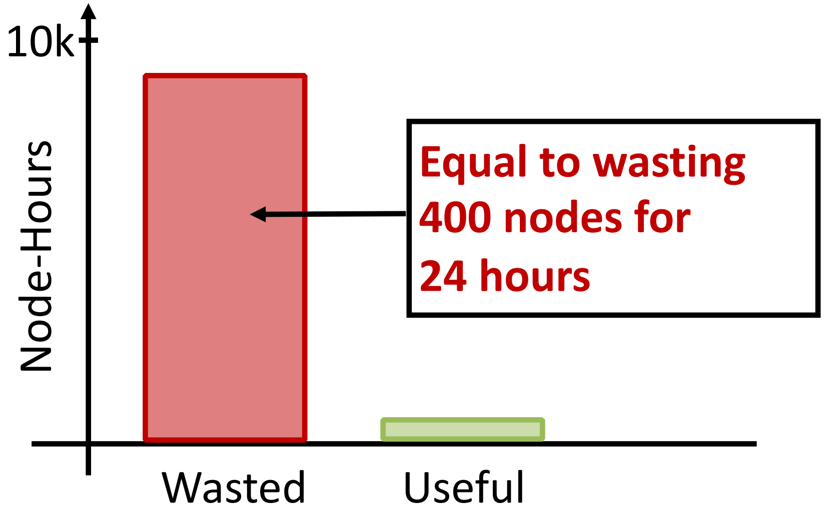


Expecting 62 messages

Sends 63 messages
DEADLOCK

Example 2:

- A non-deterministic bug in Diablo/HYPRE 2.10.1 [2]
- Application hung after several hours, in approximately 1/50 runs
- Cost of debugging effort:
  - **18 months of scientists' time**
  - **9560 node-hours**



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2. Sato, K., Ahn, D.H., Laguna, I., Lee, G.L., Schulz, M. and Chambreau, C.M., 2017, January. Noise injection techniques to expose subtle and unintended message races. In *ACM SIGPLAN Notices* (Vol. 52, No. 8, pp. 89-101). ACM.

Summary of Challenges

- HPC applications involve the interaction between:
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Our Approach

- Need to link observations of potentially harmful non-determinism to potential root causes

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- Need a metric for execution similarity
- Need a model of executions that supports such a metric

Workflow for Non-Determinism Characterization

- **Phase 1:** Build graph-structured models of executions
- **Phase 2:** Quantify cross-execution trends in non-deterministic communication via graph similarity
- **Phase 3**: Detect periods of anomalous execution dissimilarity and localize potential root causes

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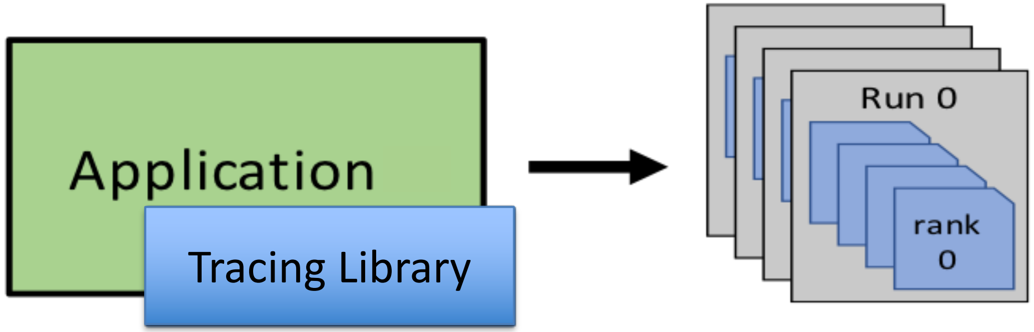
From Traces to Event Graphs



- We trace a non-deterministic application multiple times, capturing a record of communication events

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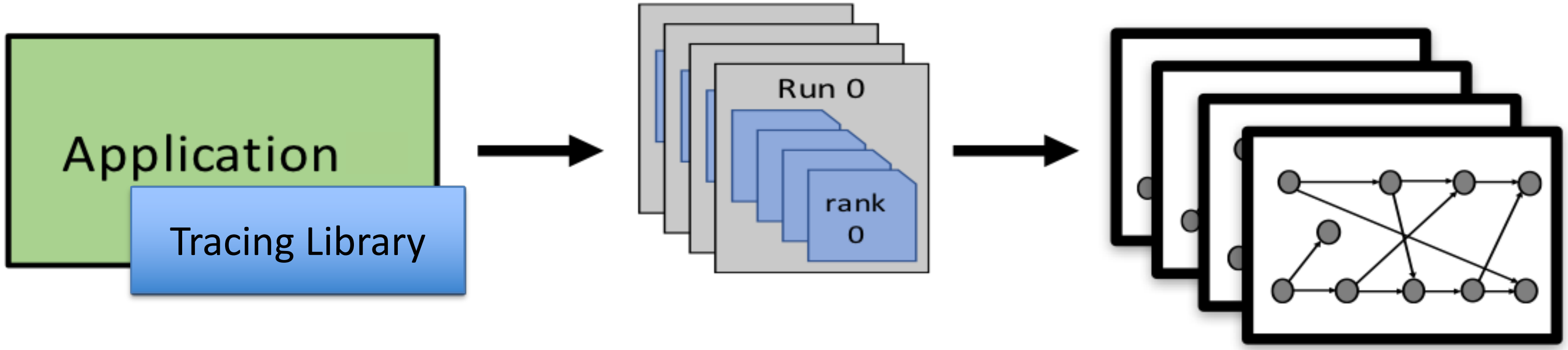

- We trace a non-deterministic application multiple times, capturing a record of communication events
- We convert the set of trace files to a graph-structured model of the inter-process communication that occurred during the execution—i.e., the event graph [3]

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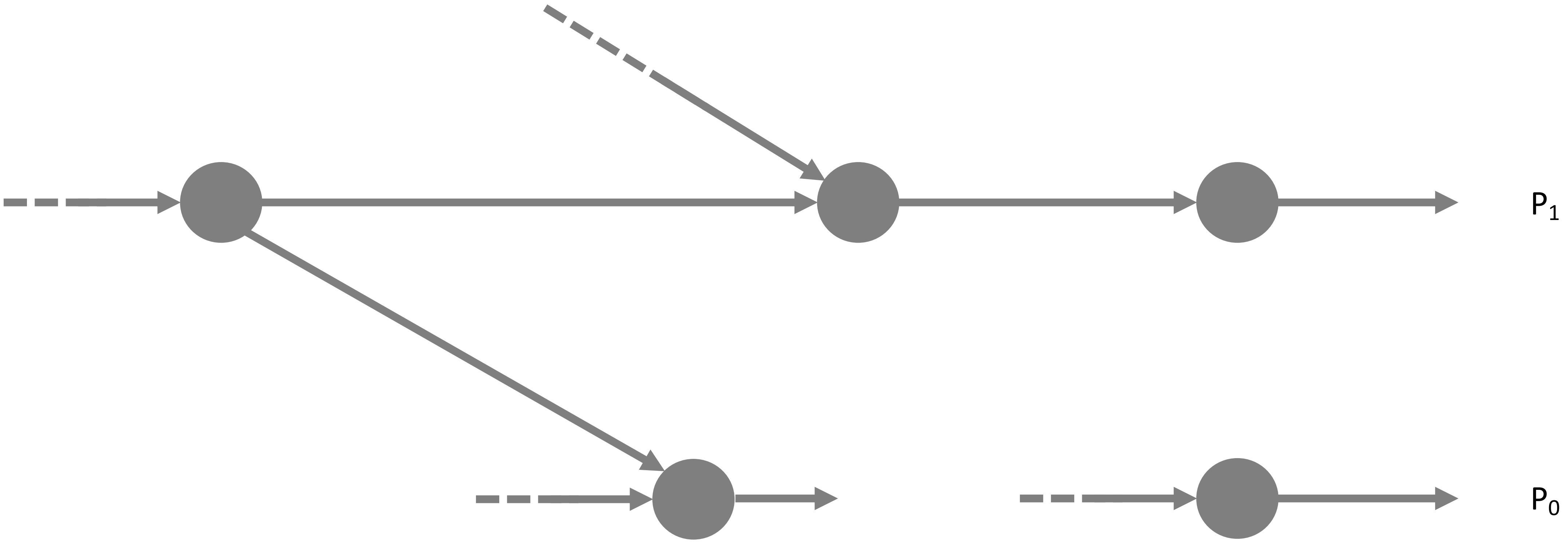
Event Graph Structure

- Directed, acyclic graph (DAG) representing a message-passing program execution [1]



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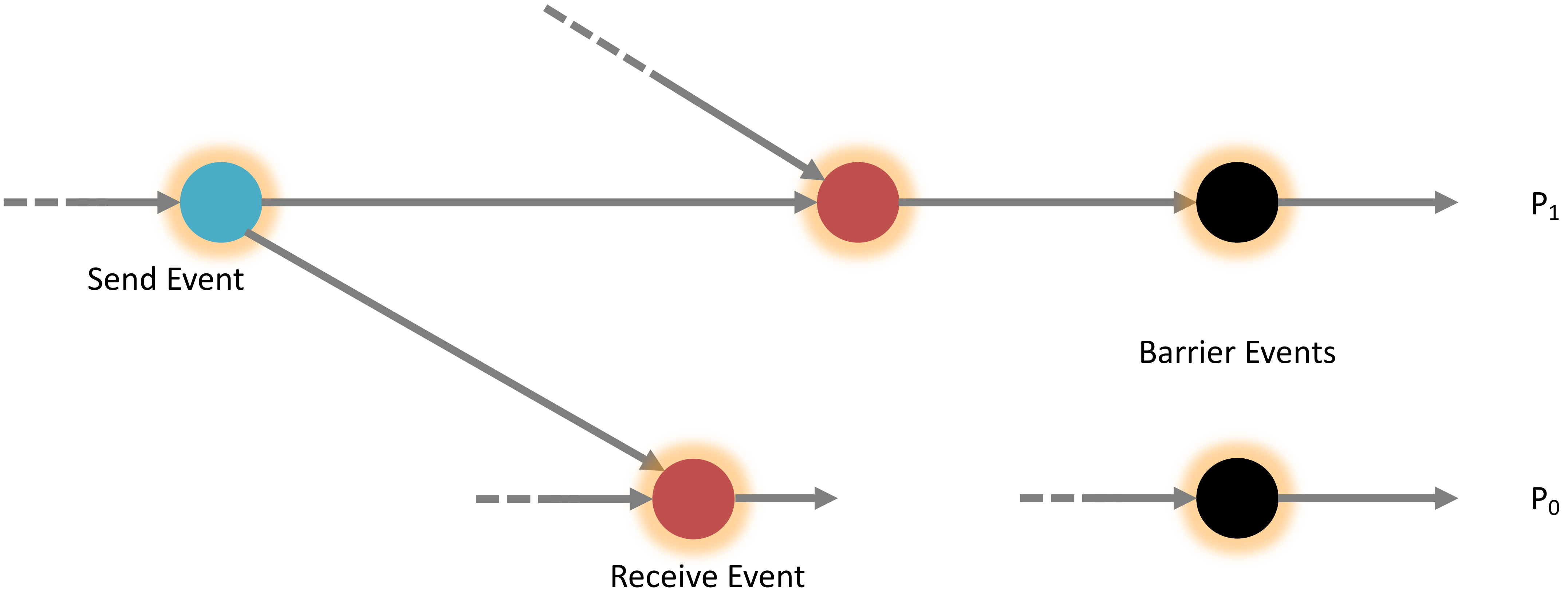

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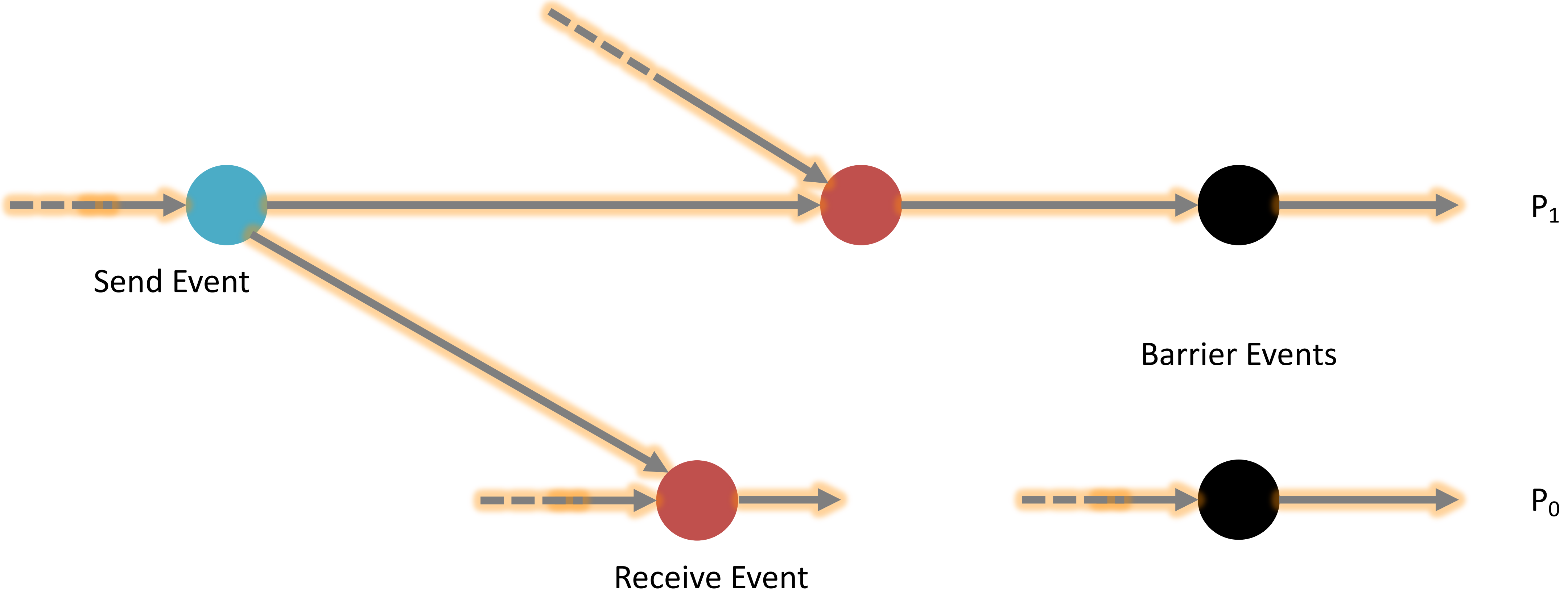
- Edges represent “happens-before”[2] relationship between events



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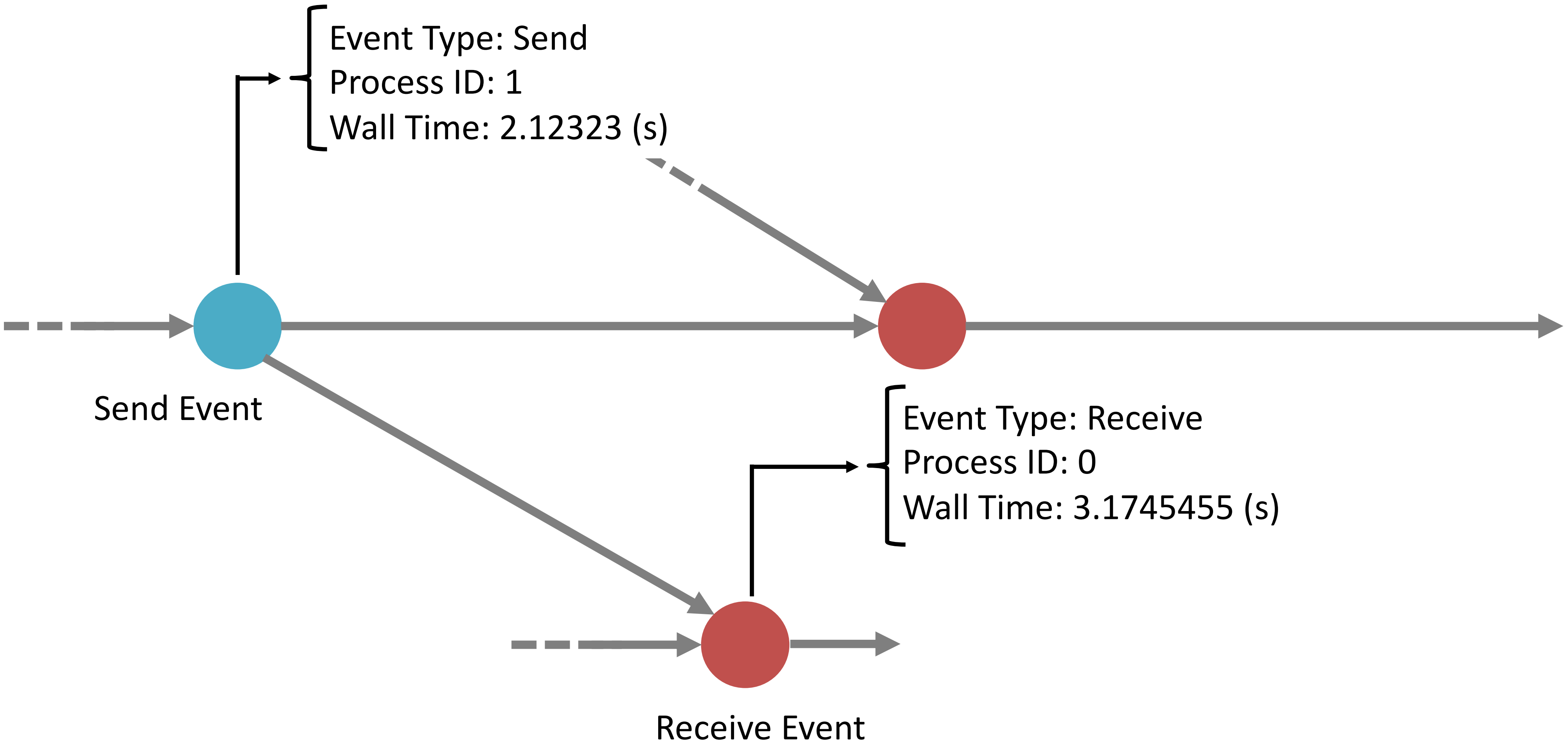
2. Lamport, L., 1978. Time, clocks, and the ordering of events in a distributed system. *Communications of the ACM*, *21*(7), pp.558-565.

Event Graph Vertex Labels



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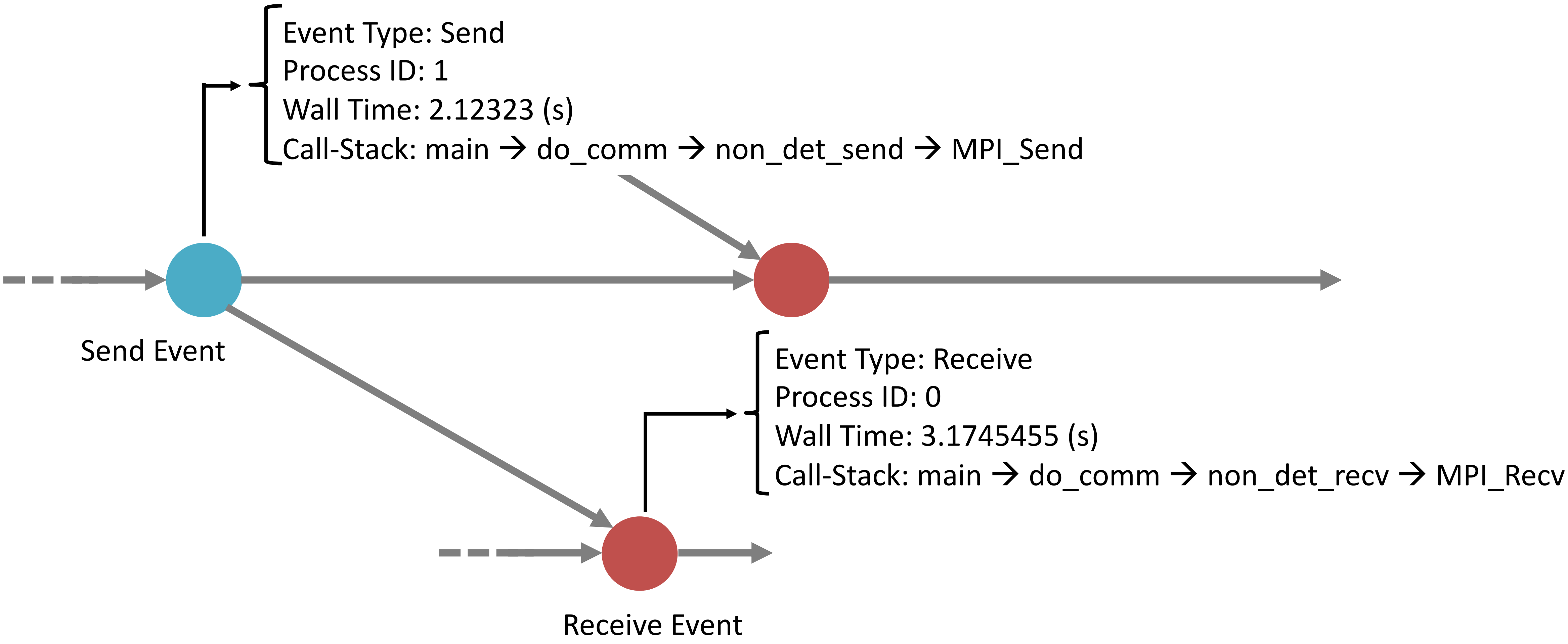
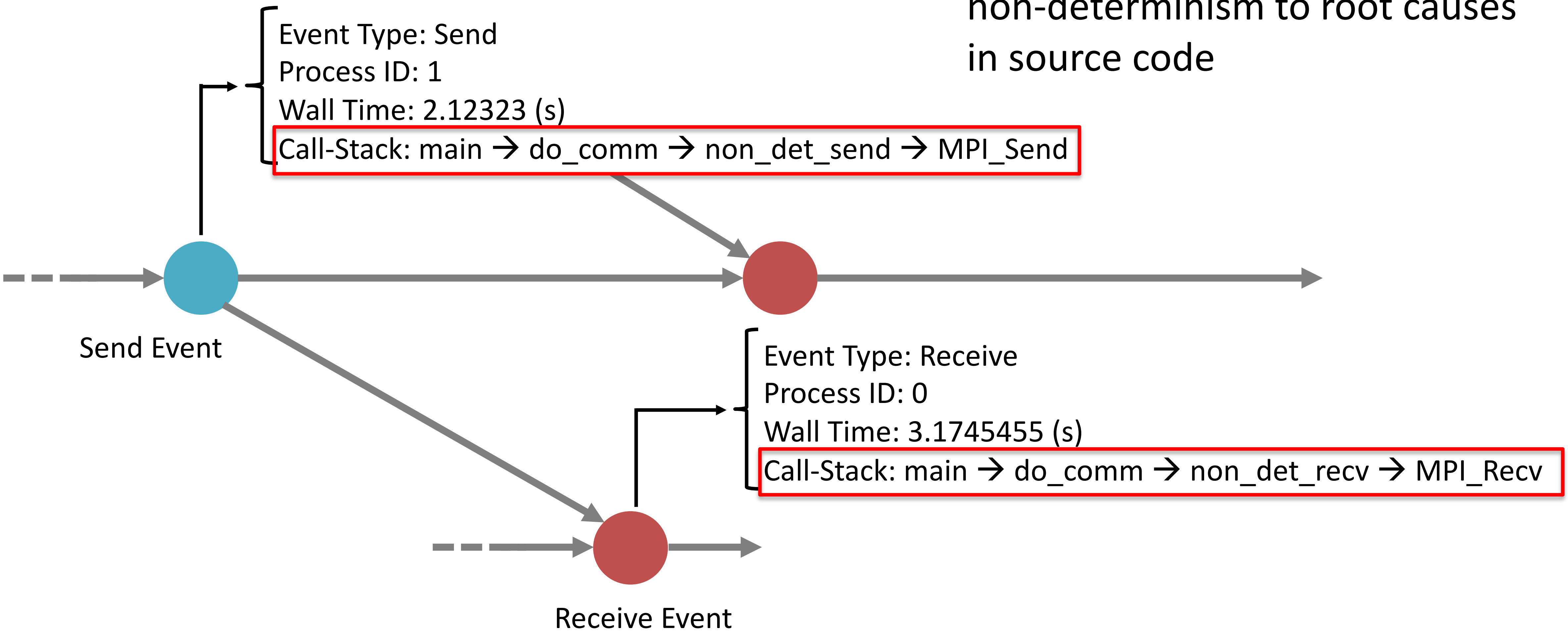


Event Graph Vertex Labels

Call-stack labels link run-time non-determinism to root causes in source code



Summary of Event Graph Model

- Traces of MPI application → DAG
- Vertices → communication events
- Edges → happens-before orders
- Vertex Labels:
  - Event type → What happened?
  - Process ID → In which process did it happen?
  - Timestamp → When did it happen?
  - Call-Stack → Where in the code did it come from?

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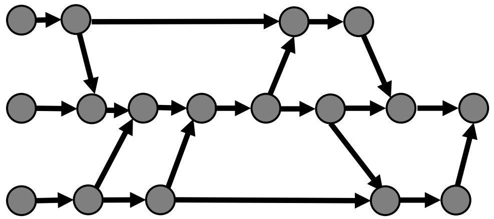
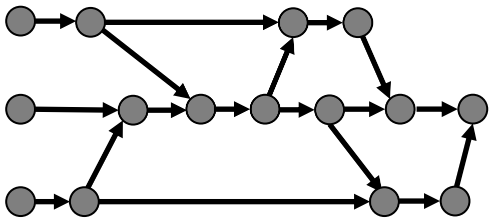
Graph Similarity via Graph Kernels

K (



,

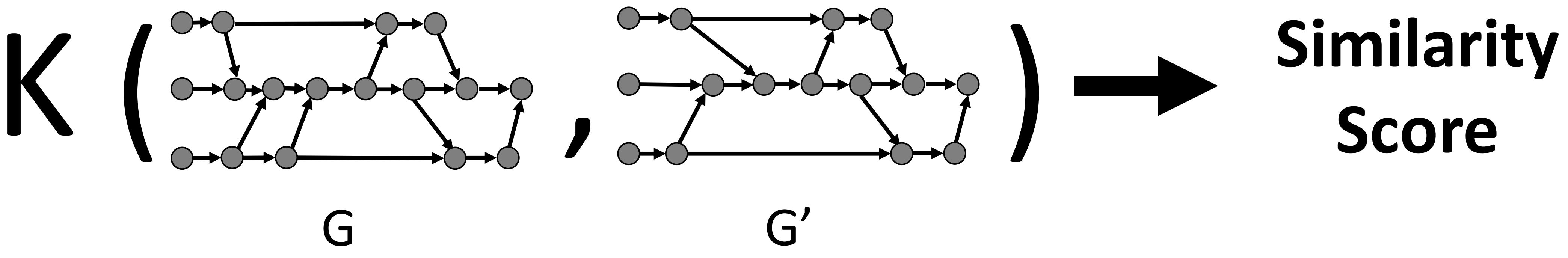


) → **Similarity Score**

G

G’

Graph Similarity via Graph Kernels



Intuition: K counts matching substructures

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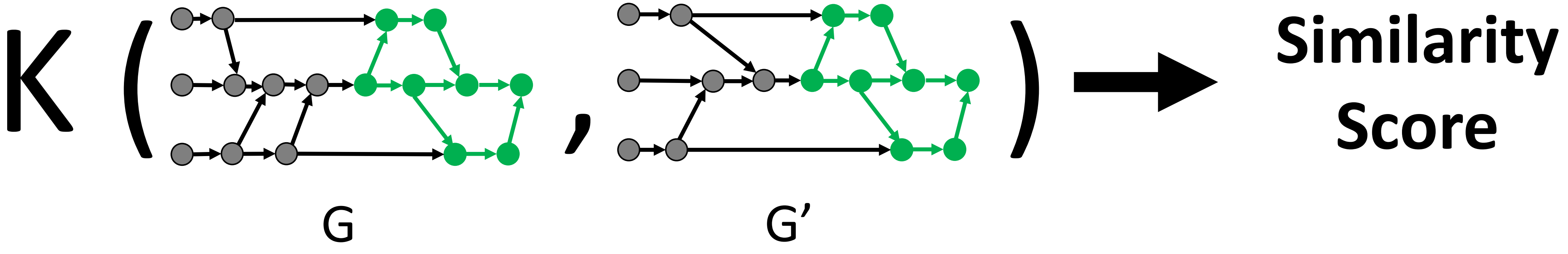

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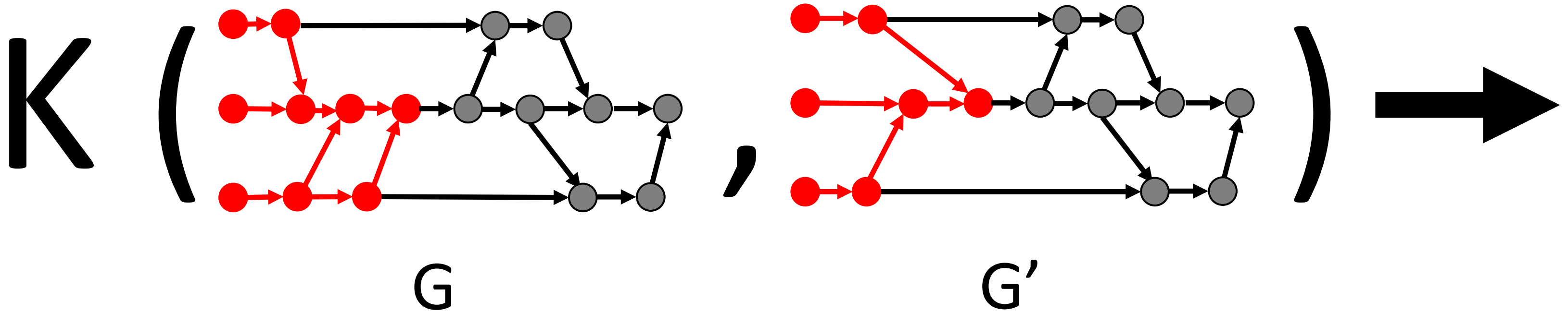

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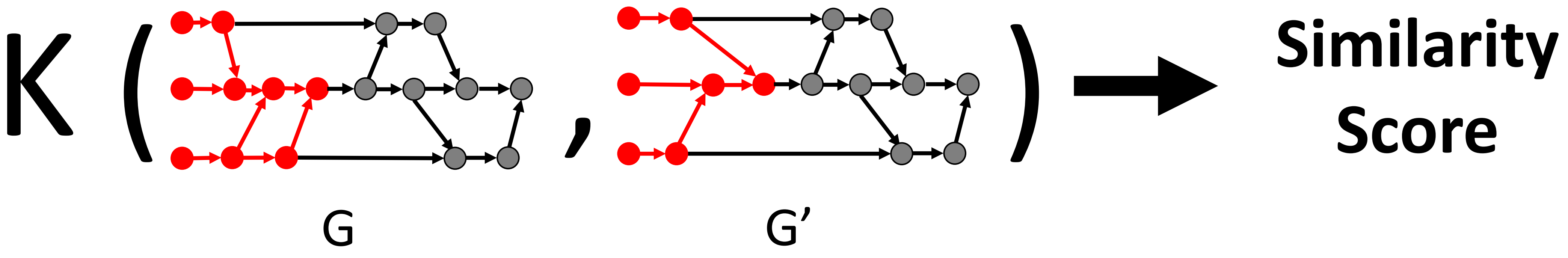

Intuition: K counts matching substructures

- Matches between G and G’ increase score
- **Differences** do not
- Graph kernel K **induces a metric** → the graph kernel distance [1]

Formula: $\mathrm{D}(\mathrm{G},\mathrm{G}') = \sqrt{K(G,G') + K(G,G') - 2K(G,G')}$

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Quantifying Non-Determinism via Graph Kernel Distance

We evaluate the Weisfeiler-Lehman Subtree Pattern Kernel for quantifying dissimilarity between event graphs:

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- Incorporation of arbitrary vertex label data

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Kernel Distance Evaluation Methodology

- Construct event graphs for common communication patterns with:
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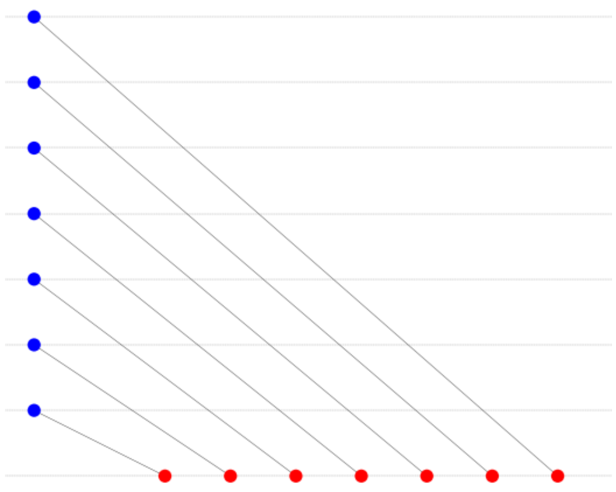
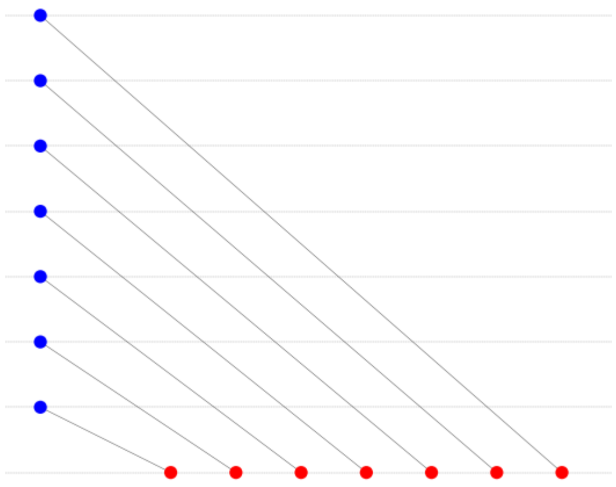
- Construct event graphs for common communication patterns with:
  - Controlled degree of non-determinism
  - Fixed amount of communication volume
- **Hypothesis:** As greater non-determinism is permitted in the runs, the graph kernel distances between the event graphs representing those runs will increase

Run 1

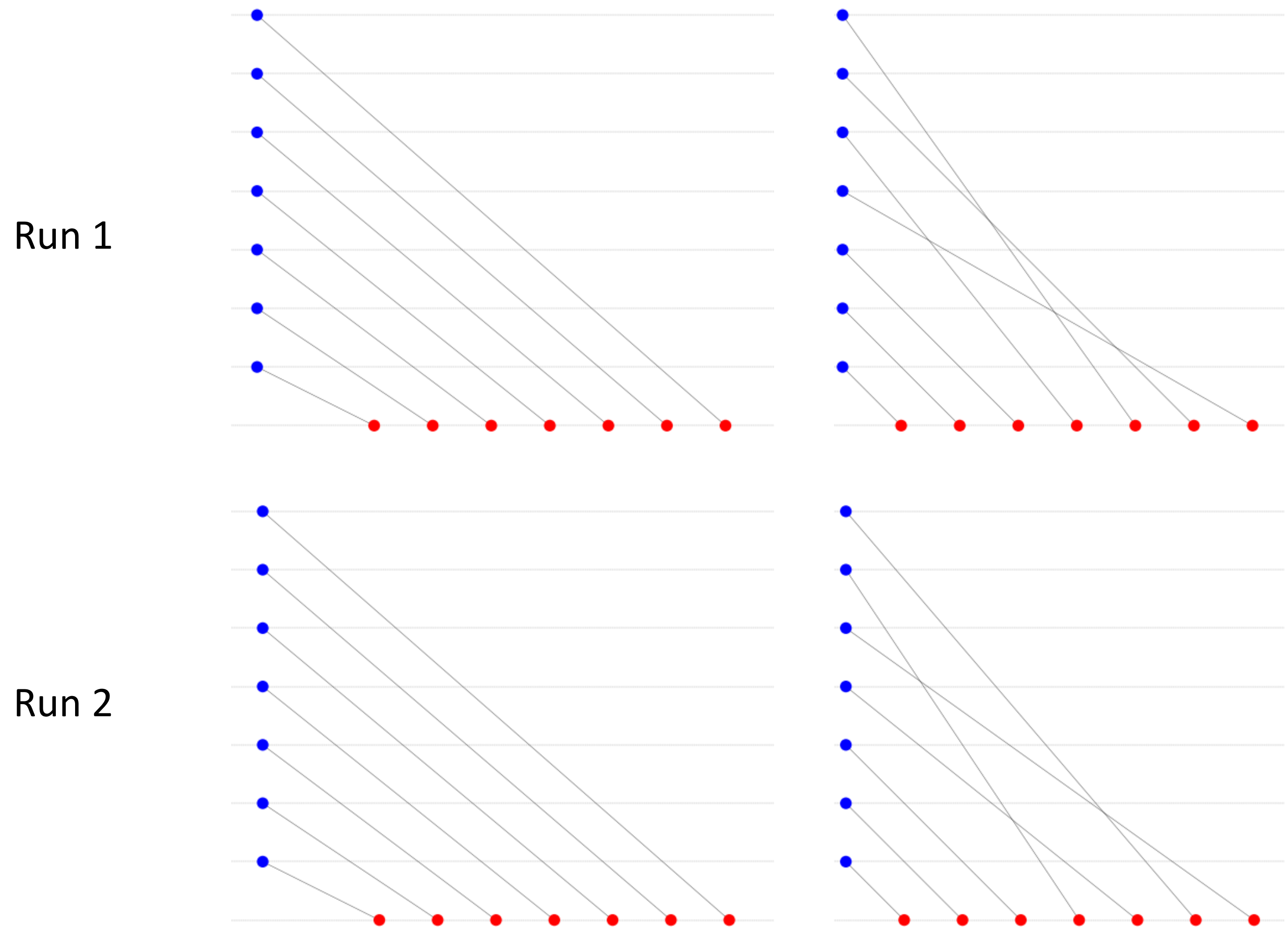


Run 2



Deterministic

All receives guaranteed to occur
in same order run-to-run



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Partially Non-Deterministic

Some receives guaranteed to occur in same order

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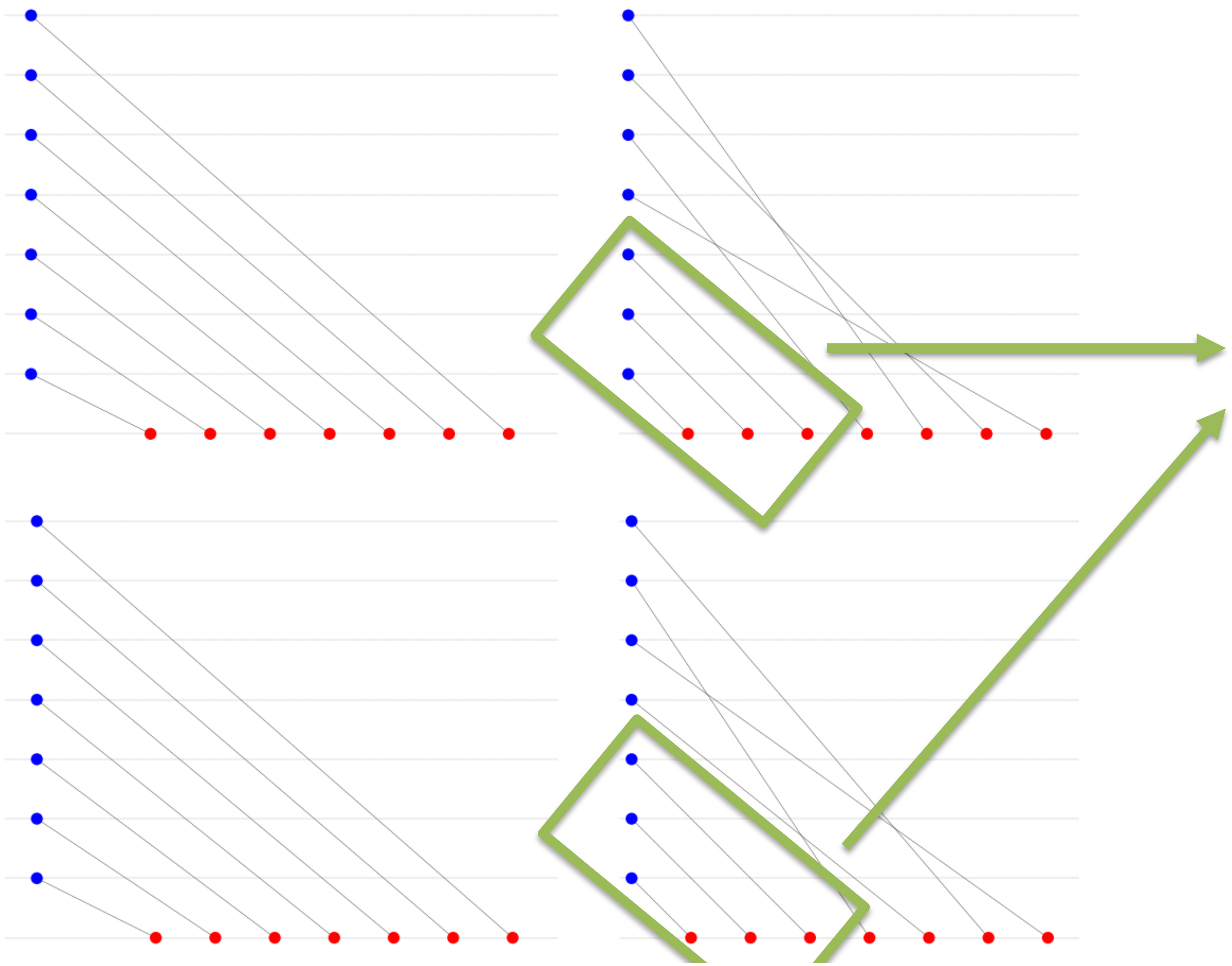
Run 2



These messages are always received in same order

<u>Deterministic</u>

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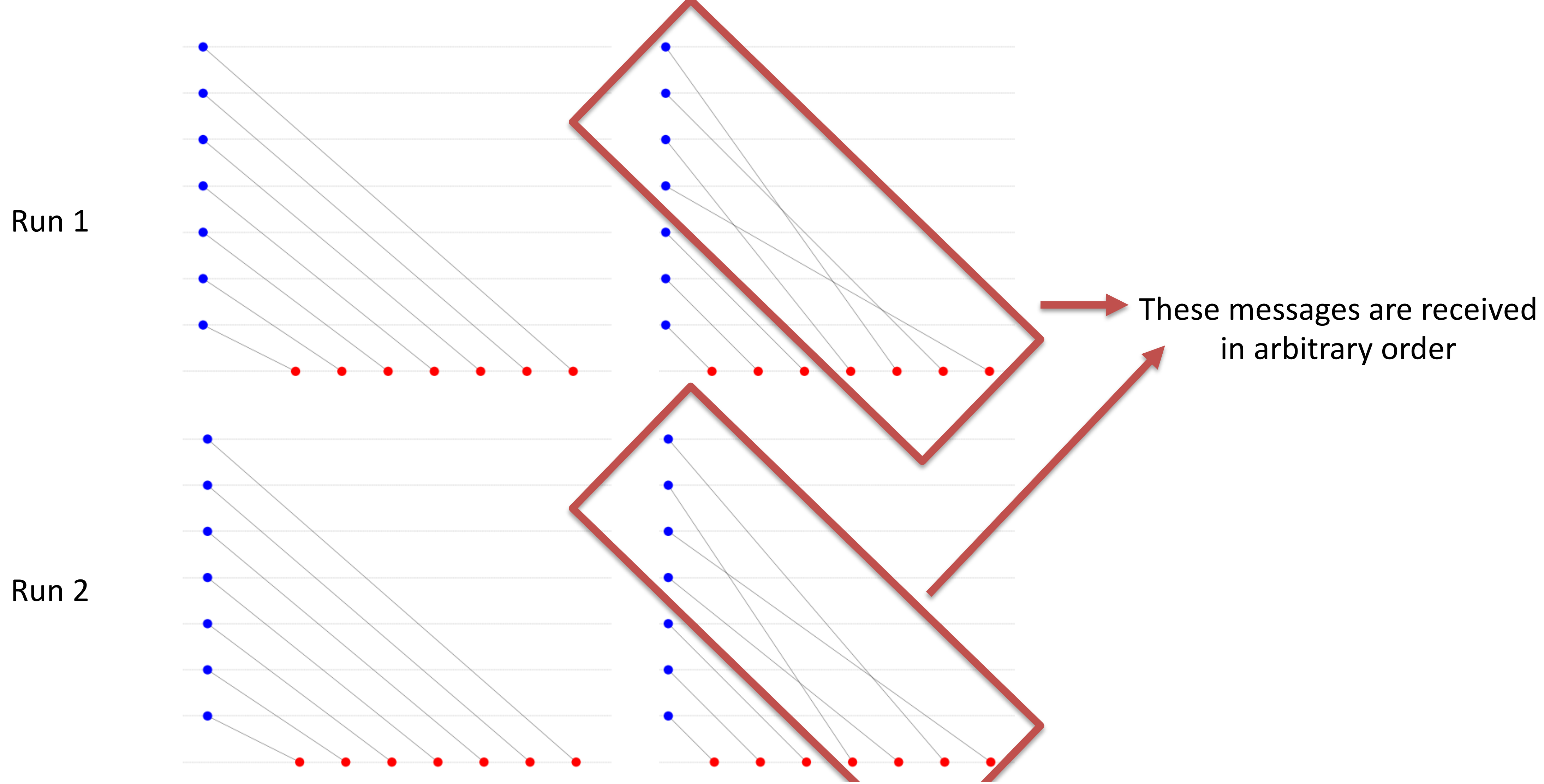
<u>Partially Non-Deterministic</u>

Some receives guaranteed to occur in same order



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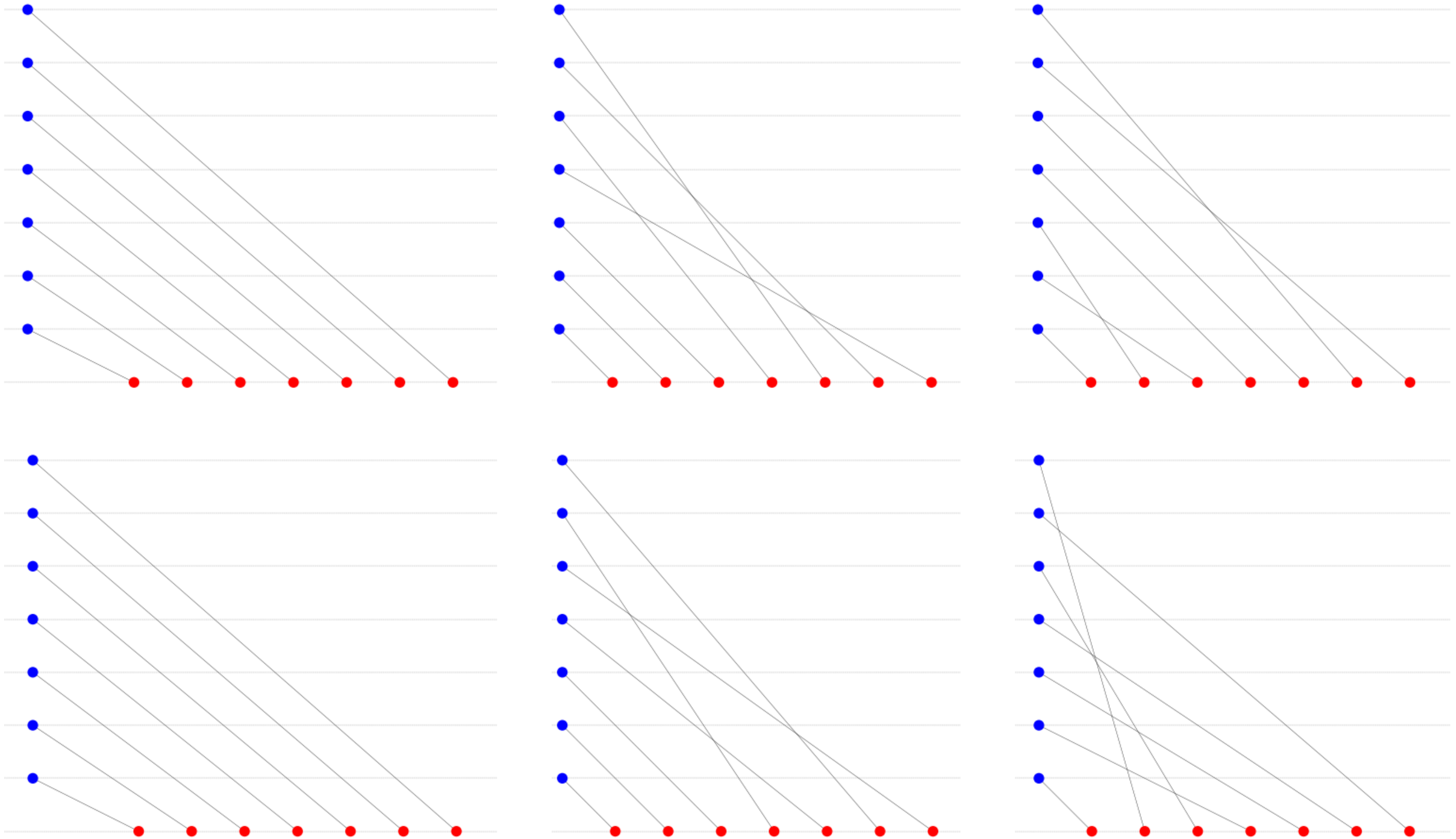
Run 2



Deterministic

All receives guaranteed to occur in same order run-to-run

Partially Non-Deterministic

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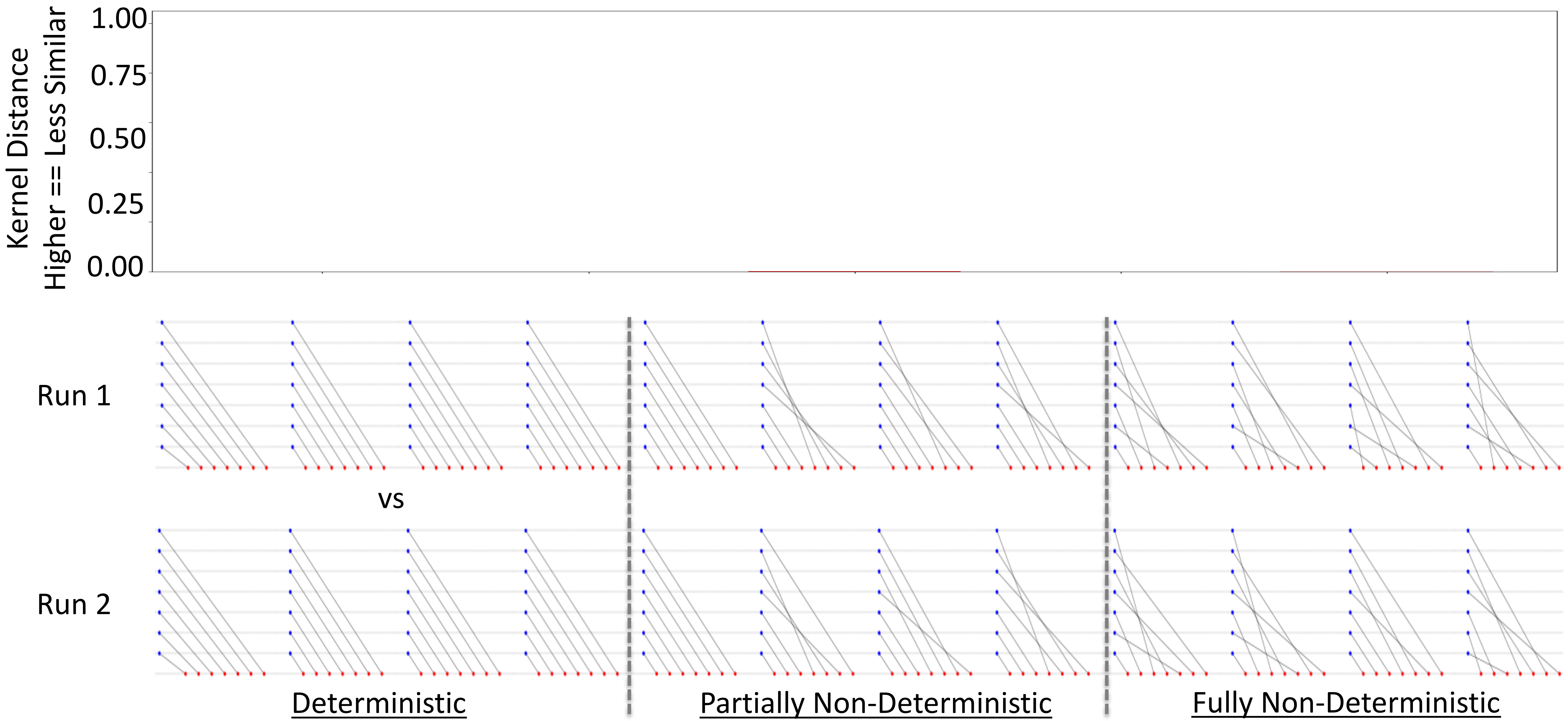
Fully Non-Deterministic

All receives occur in arbitrary order run-to-run

Comparing Runs via Kernel Distance



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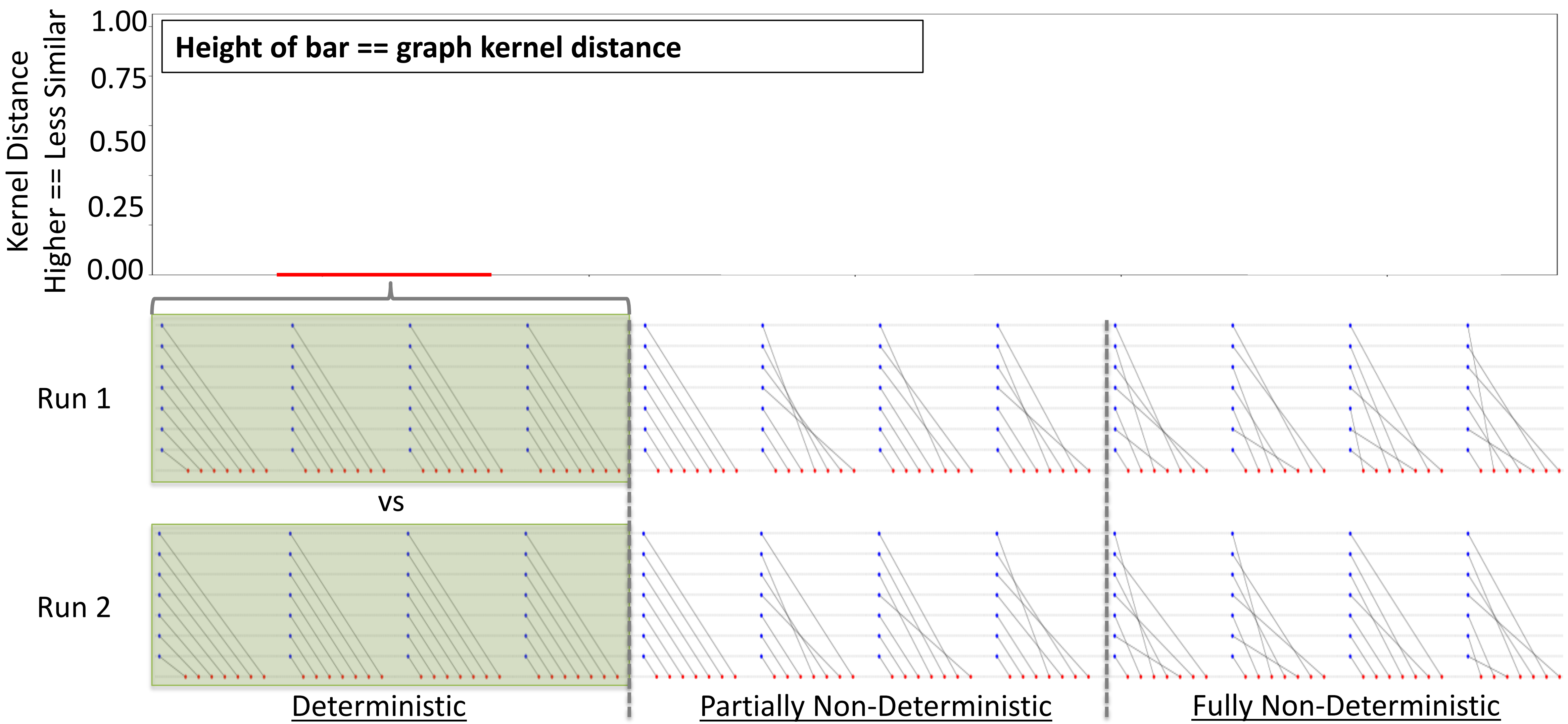

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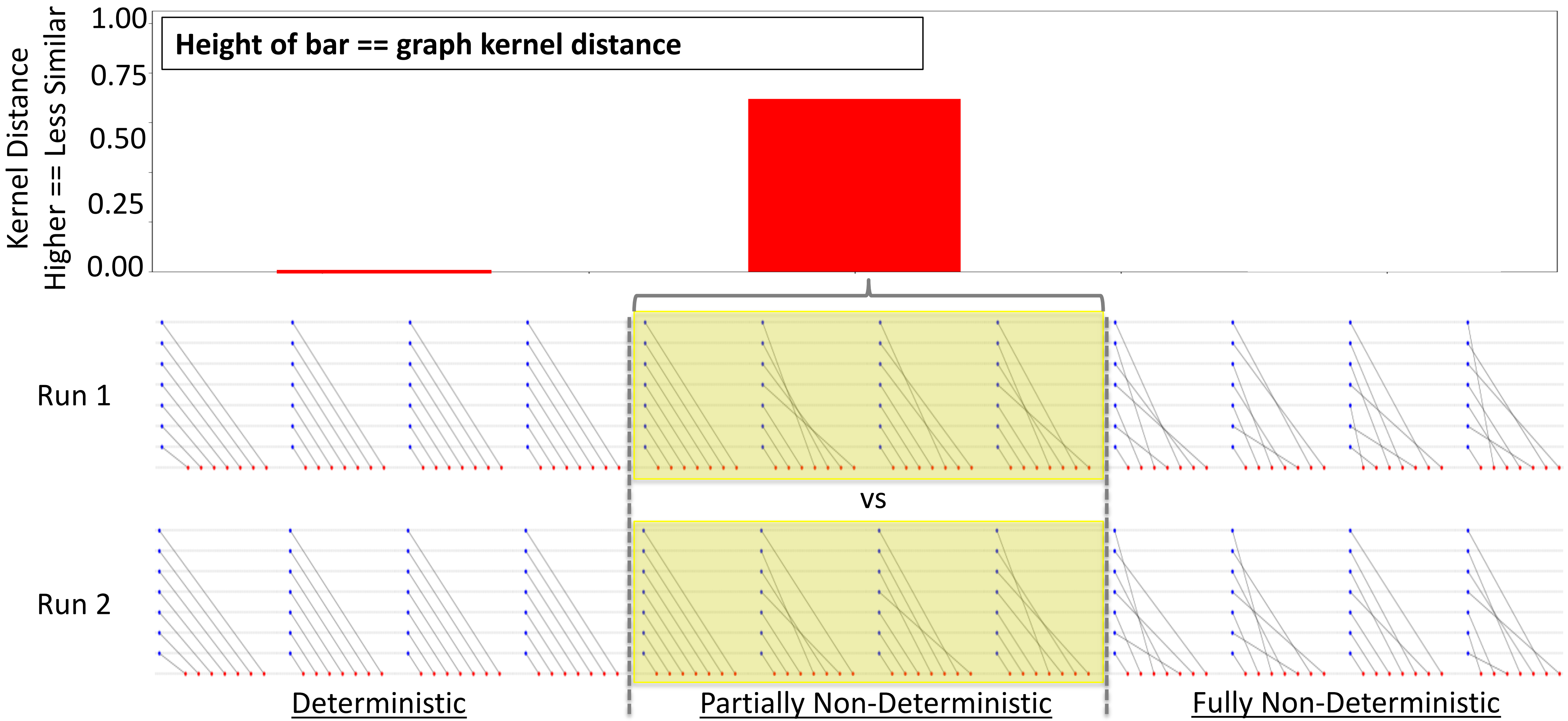

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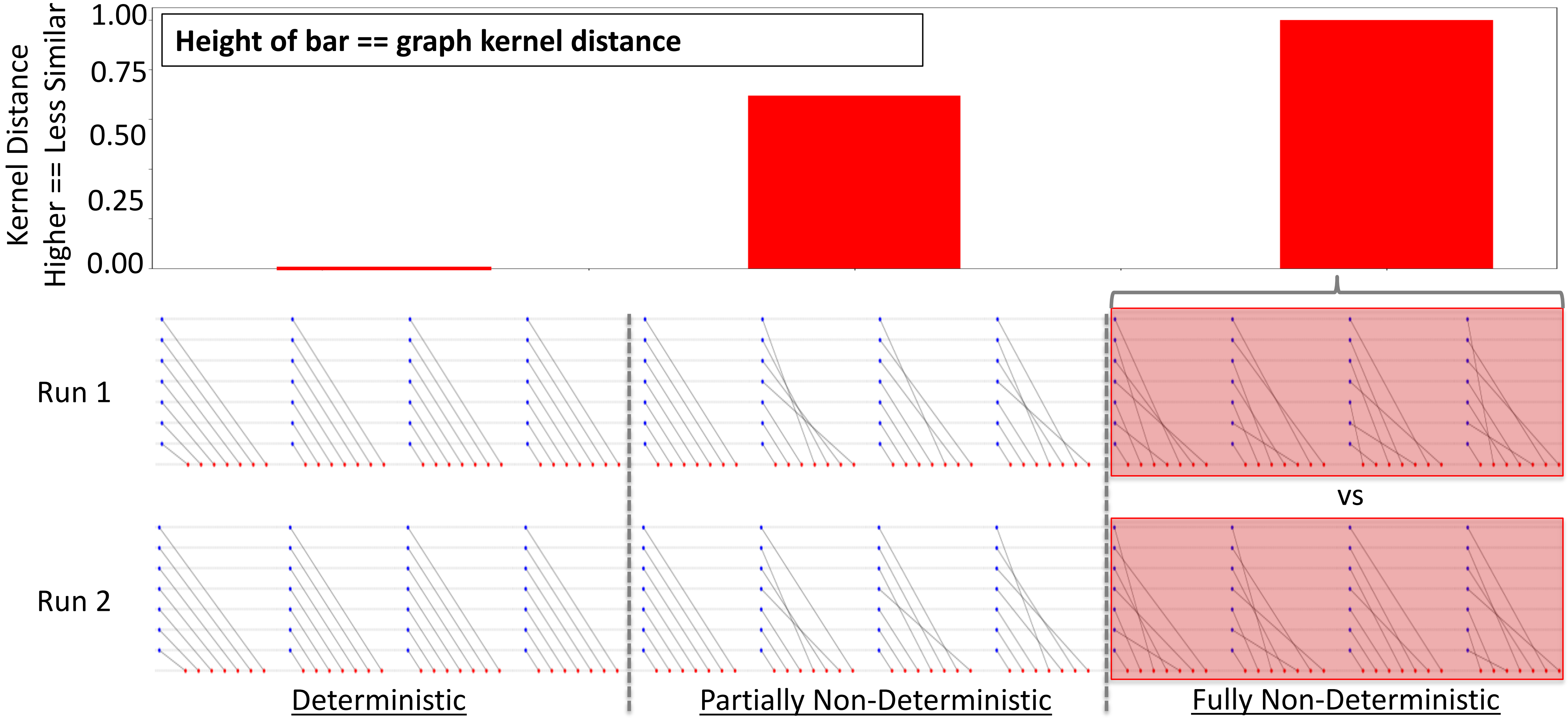


Kernel Distance Trends Across Multiple Runs

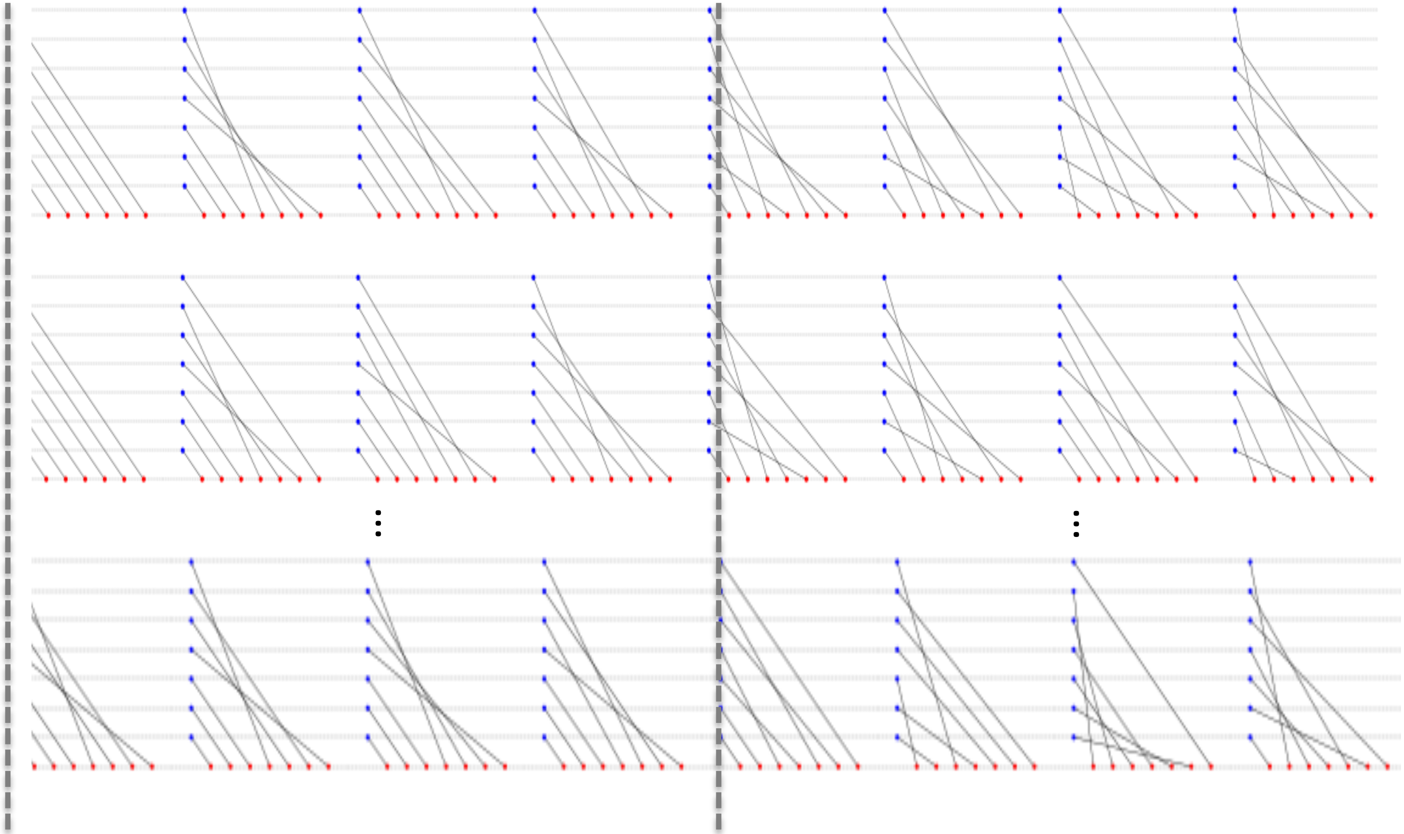
- Previous example only measured kernel distance between two executions
- But we want a statistical picture of the **trend in kernel distance over time across many executions**

Run 1

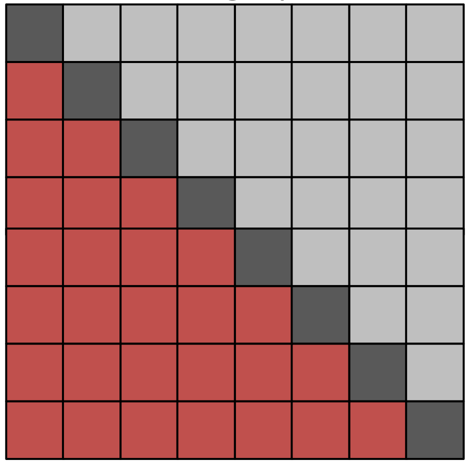
Run 2

⋮

Run N



Kernel matrix
w/r/t chosen graph kernel K

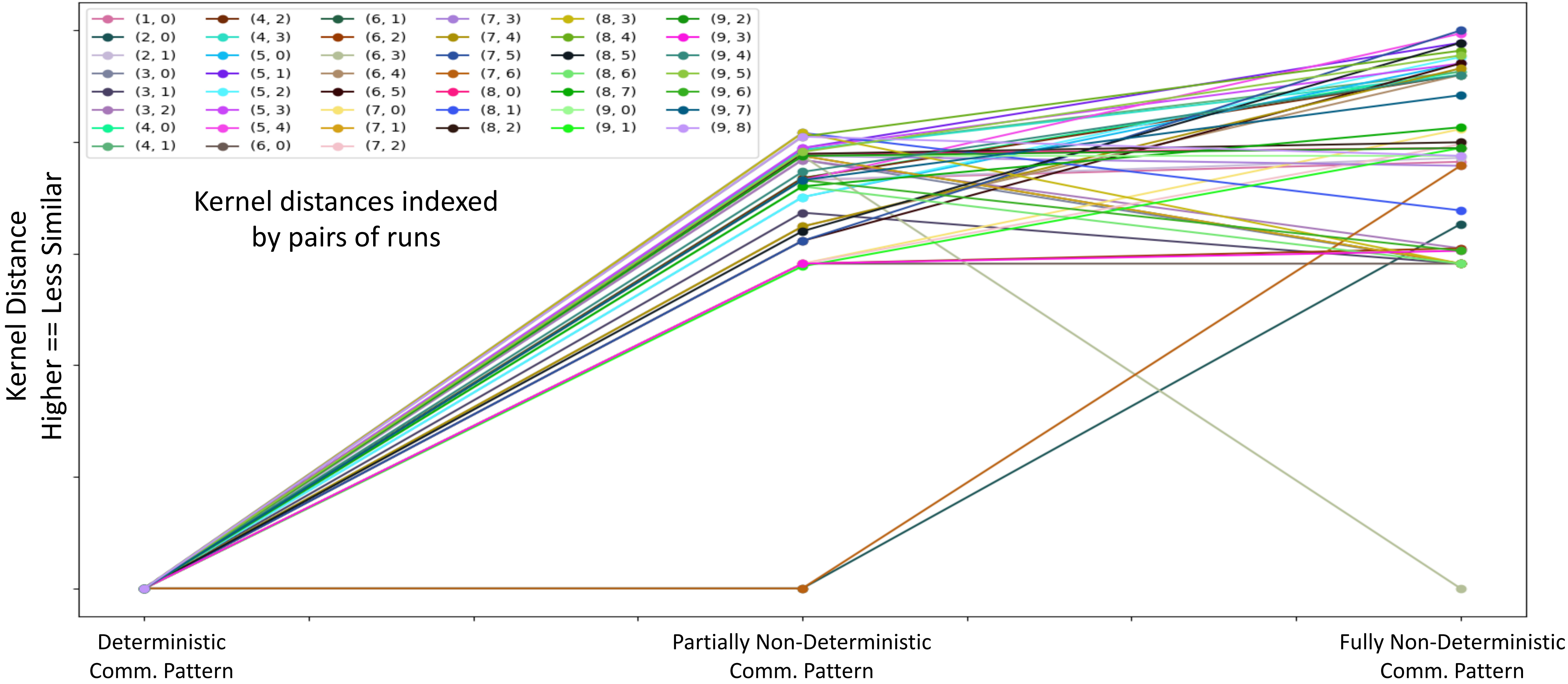


= kernel distance between graphs i and j

= kernel distance from graph to itself, always 0

= redundant, due to symmetry

Kernel Distance Trends Across Multiple Runs



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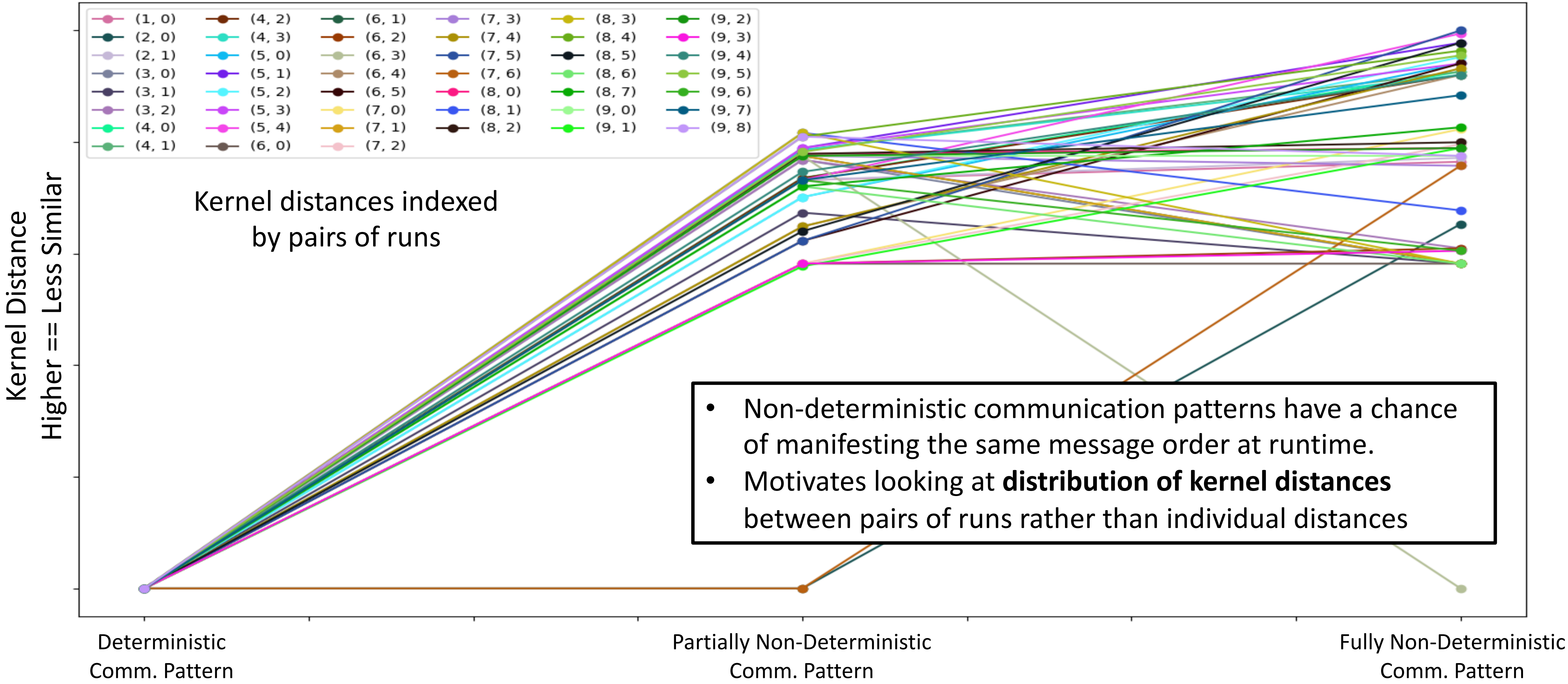

- Non-deterministic communication patterns have a chance of manifesting the same message order at runtime.
- Motivates looking at **distribution of kernel distances** between pairs of runs rather than individual distances

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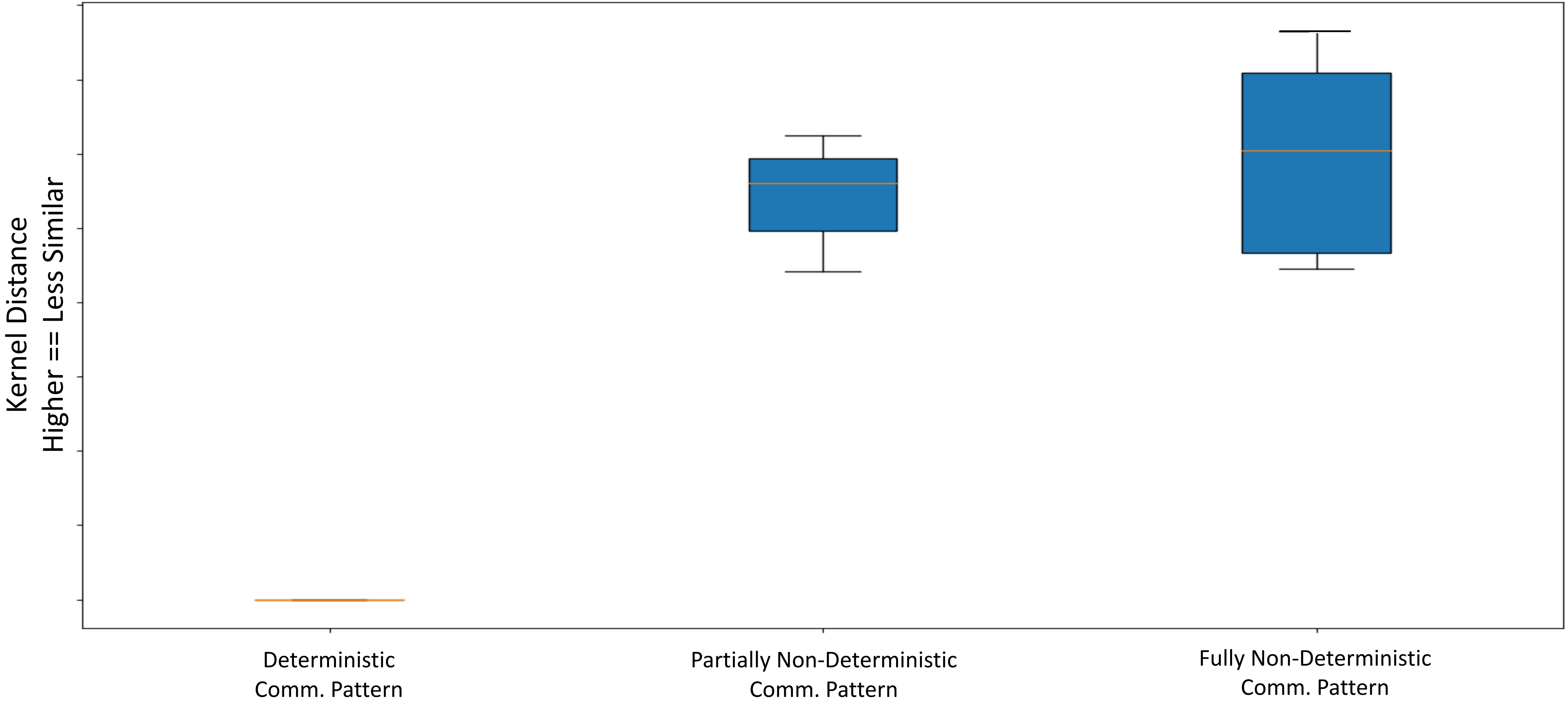

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1. Cappello, F., Guermouche, A. and Snir, M., 2010, August. On communication determinism in parallel HPC applications. In *2010 Proceedings of 19th International Conference on Computer Communications and Networks* (pp. 1-8). IEEE.

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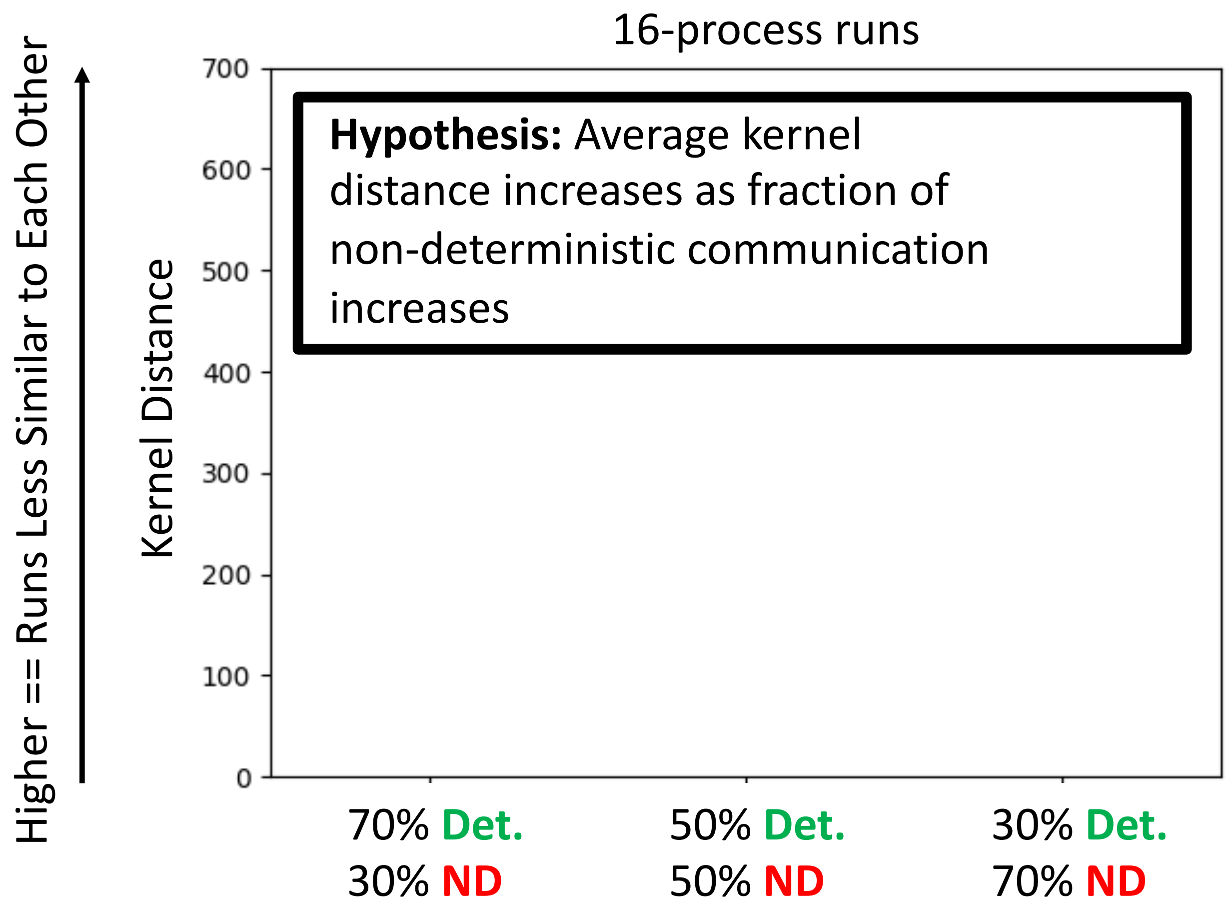
- Known to exhibit both receiver-side non-determinism and sender-side non-determinism [1]
- For our evaluation, we control proportion of non-deterministic communication volume by splitting ranks into two groups:
  - One group performs the actual non-deterministic AMG pattern
  - One group performs a determinized version of the pattern

1. Cappello, F., Guermouche, A. and Snir, M., 2010, August. On communication determinism in parallel HPC applications. In *2010 Proceedings of 19th International Conference on Computer Communications and Networks* (pp. 1-8). IEEE.

Kernel Distance Between Runs of Sequoia-AMG



Graph Kernel Used: Weisfeiler-Lehman Subtree Kernel [1]

1. Shervashidze, N., Schweitzer, P., Leeuwen, E.J.V., Mehlhorn, K. and Borgwardt, K.M., 2011. Weisfeiler-lehman graph kernels. *Journal of Machine Learning Research*, *12*(Sep), pp.2539-2561.

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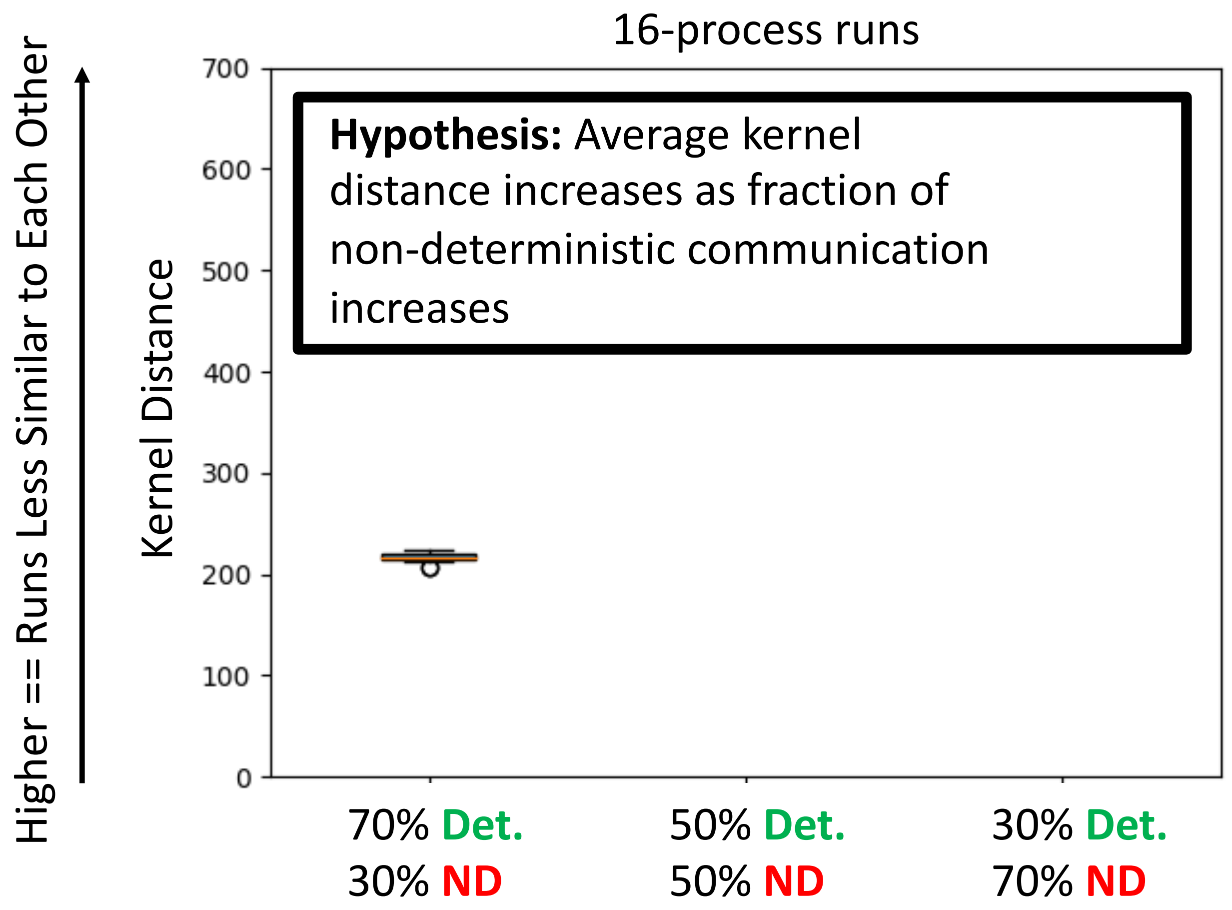

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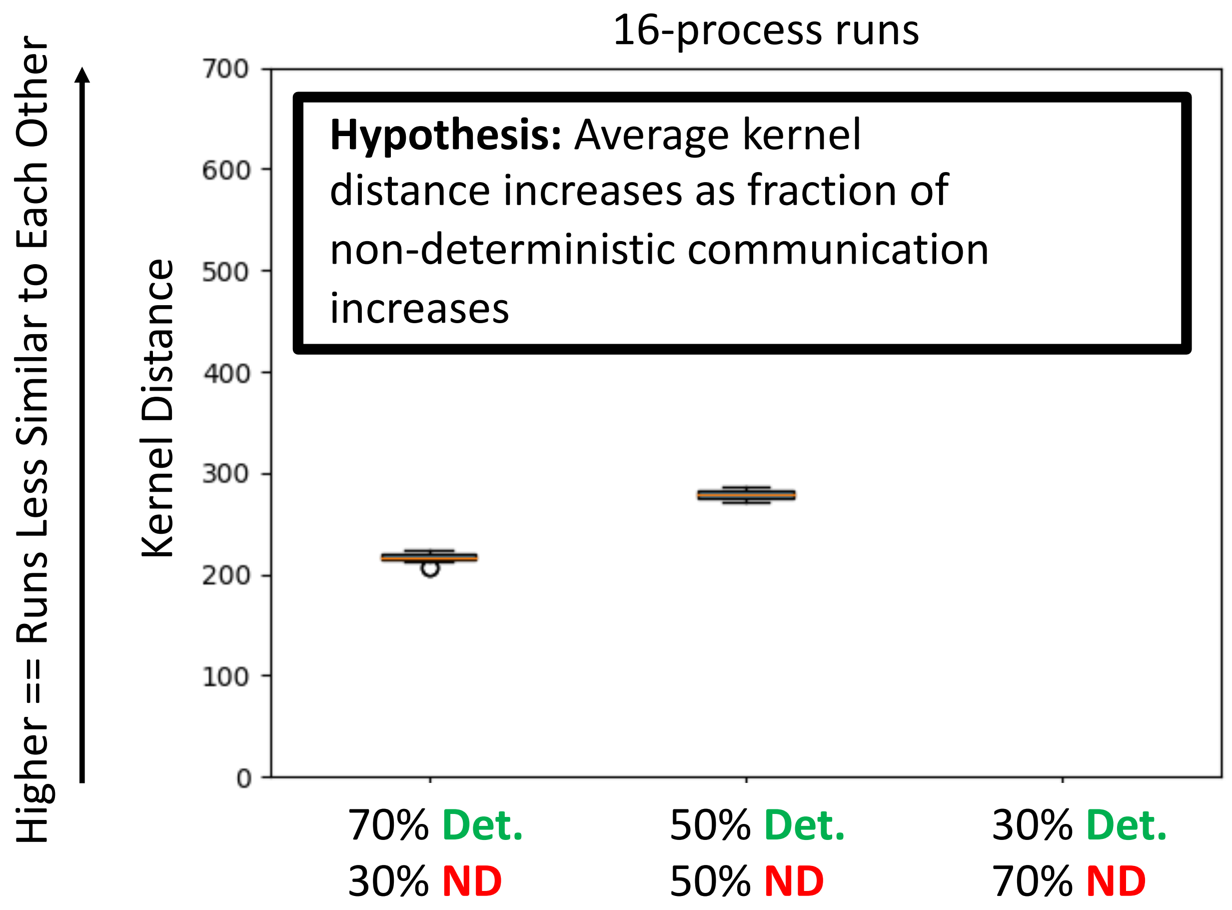

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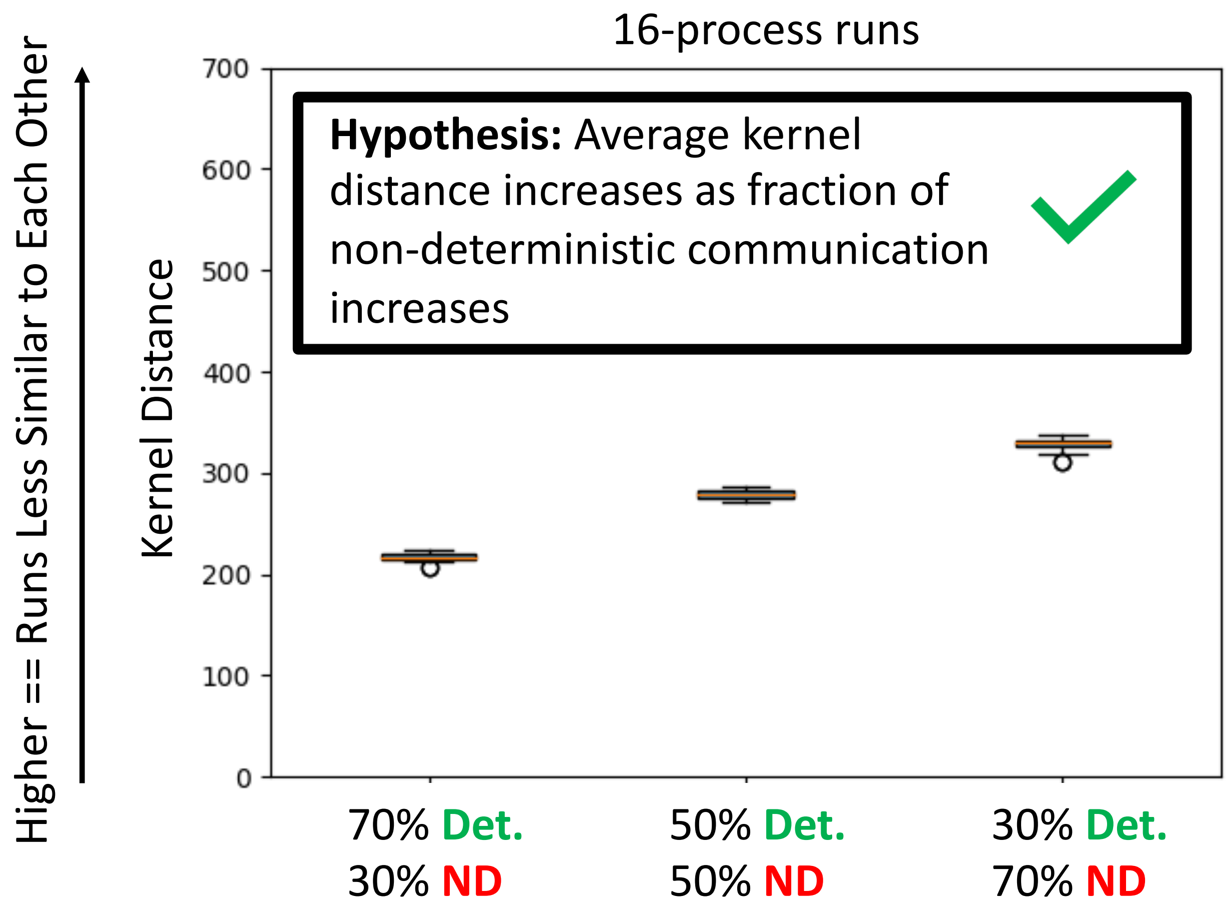

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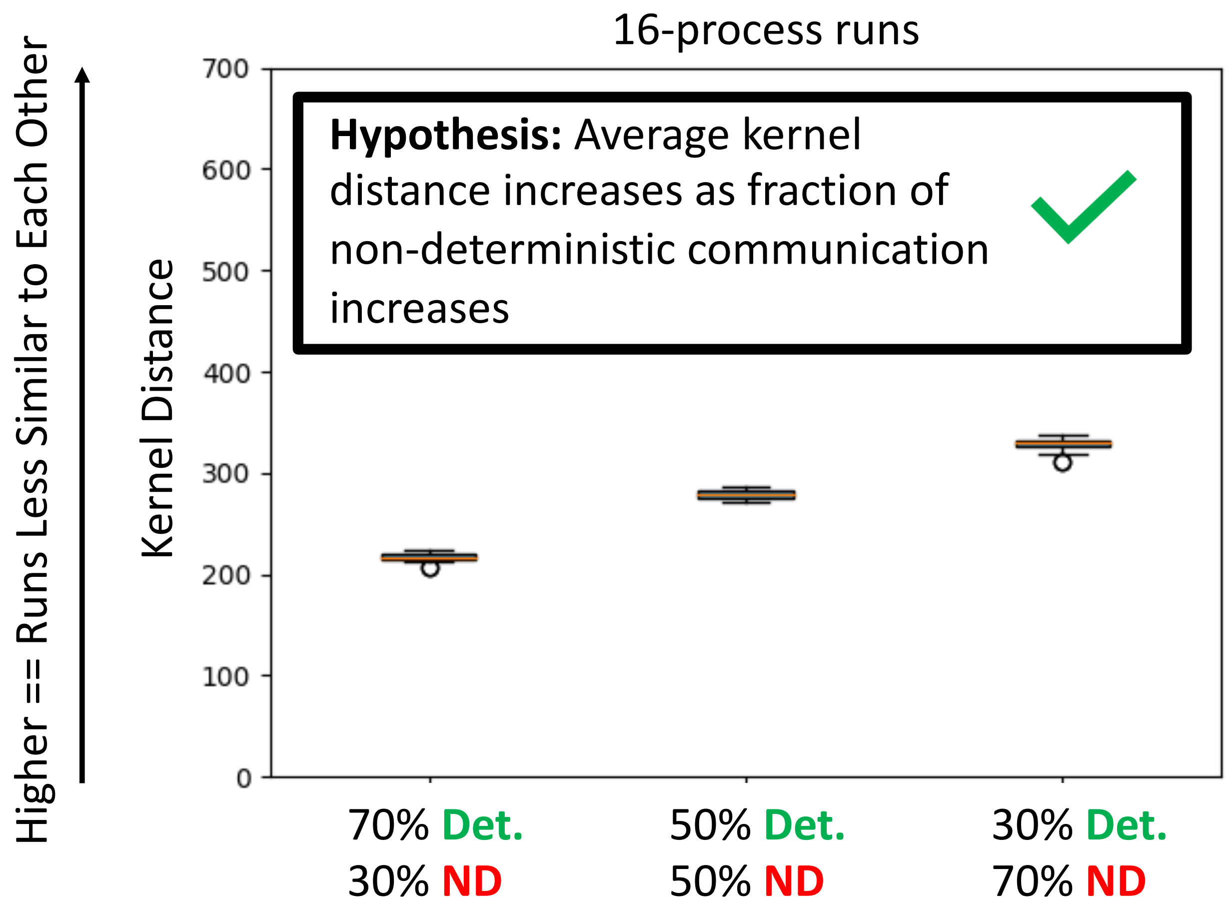

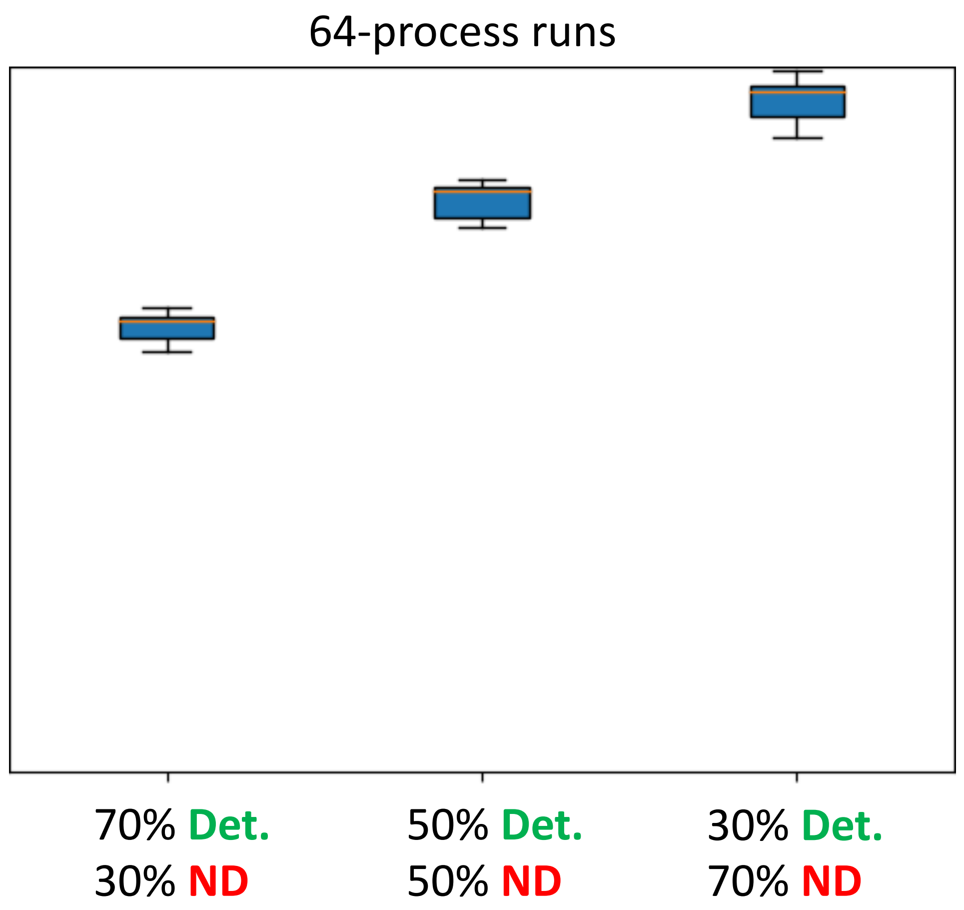

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Lessons Learned

- Graph kernel distance is a useful proxy for degree of non-determinism in a communication pattern

Lessons Learned

- Graph kernel distance is a useful proxy for degree of non-determinism in a communication pattern
- This holds for both:
  - Simple communication patterns with only receiver-side non-determinism (e.g., naïve reduce pattern)
  - More complex patterns with mixed receiver/sender-side non-determinism (e.g., Sequoia-AMG Iprobe pattern)

Workflow for Non-Determinism Characterization

- **Phase 1:** Build graph-structured models of executions
- **Phase 2:** Quantify cross-execution trends in non-deterministic communication via graph similarity
- **Phase 3**: Detect periods of anomalous execution dissimilarity and localize potential root causes

Applying our Workflow to miniAMR

- Adaptive mesh refinement (AMR) code from the Matevo Benchmark Suite [1]

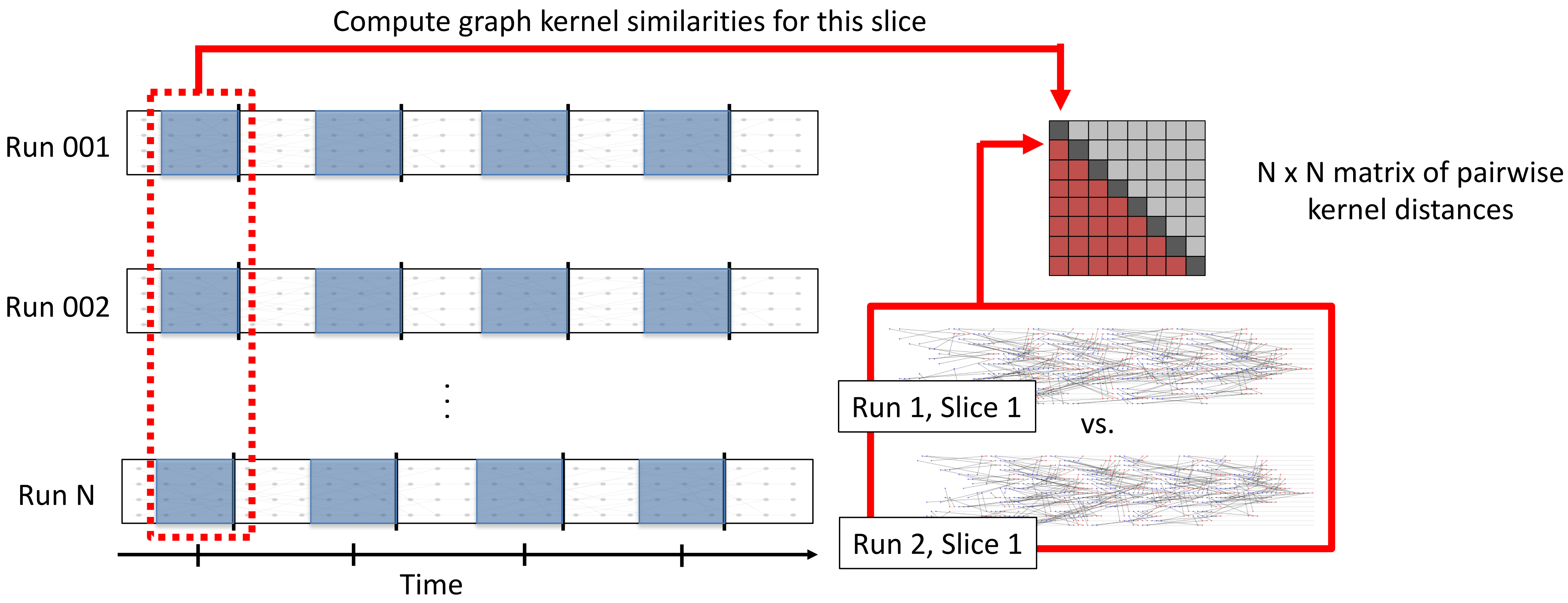
1. Heroux, M.A., Doerfler, D.W., Crozier, P.S., Willenbring, J.M., Edwards, H.C., Williams, A., Rajan, M., Keiter, E.R., Thornquist, H.K. and Numrich, R.W., 2009. Improving performance via mini-applications. *Sandia National Laboratories, Tech. Rep. SAND2009-5574*, *3*.

Applying our Workflow to miniAMR

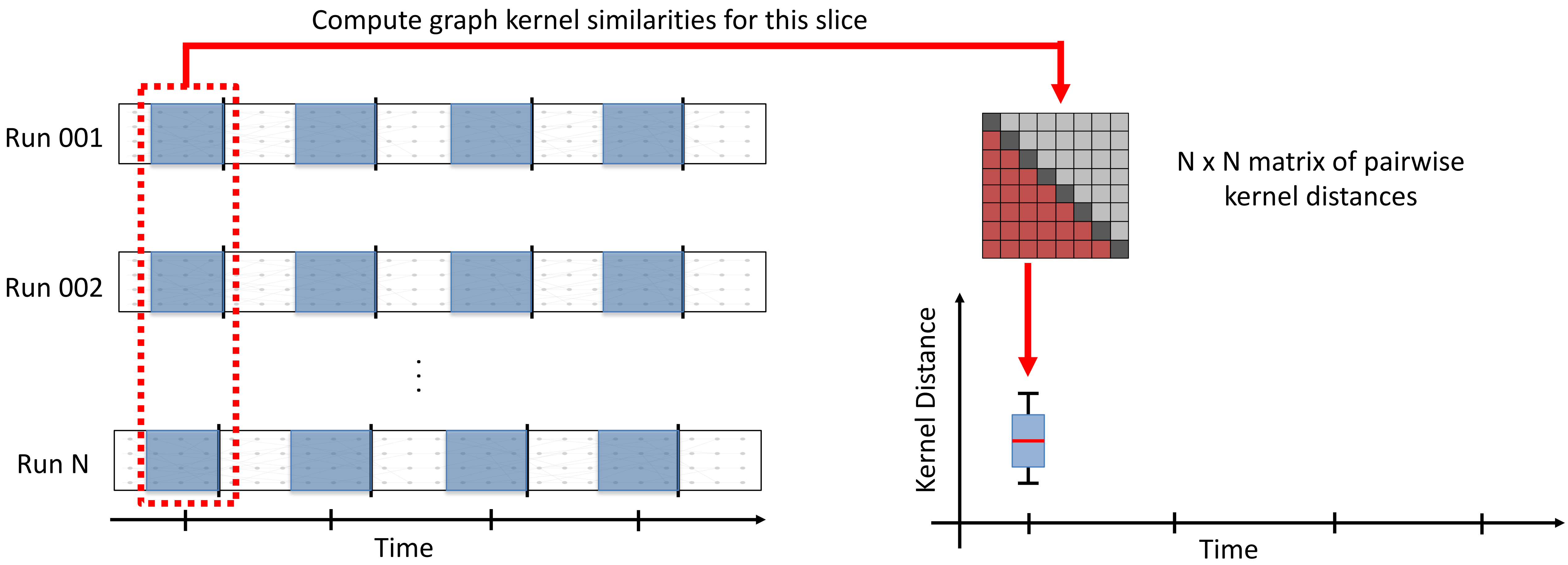
- Adaptive mesh refinement (AMR) code from the Matevo Benchmark Suite [1]
- We target miniAMR based on the following criteria:
  - MPI application exhibiting communication non-determinism
  - Root cause of non-determinism known *a priori*

1. Heroux, M.A., Doerfler, D.W., Crozier, P.S., Willenbring, J.M., Edwards, H.C., Williams, A., Rajan, M., Keiter, E.R., Thornquist, H.K. and Numrich, R.W., 2009. Improving performance via mini-applications. *Sandia National Laboratories, Tech. Rep. SAND2009-5574*, *3*.

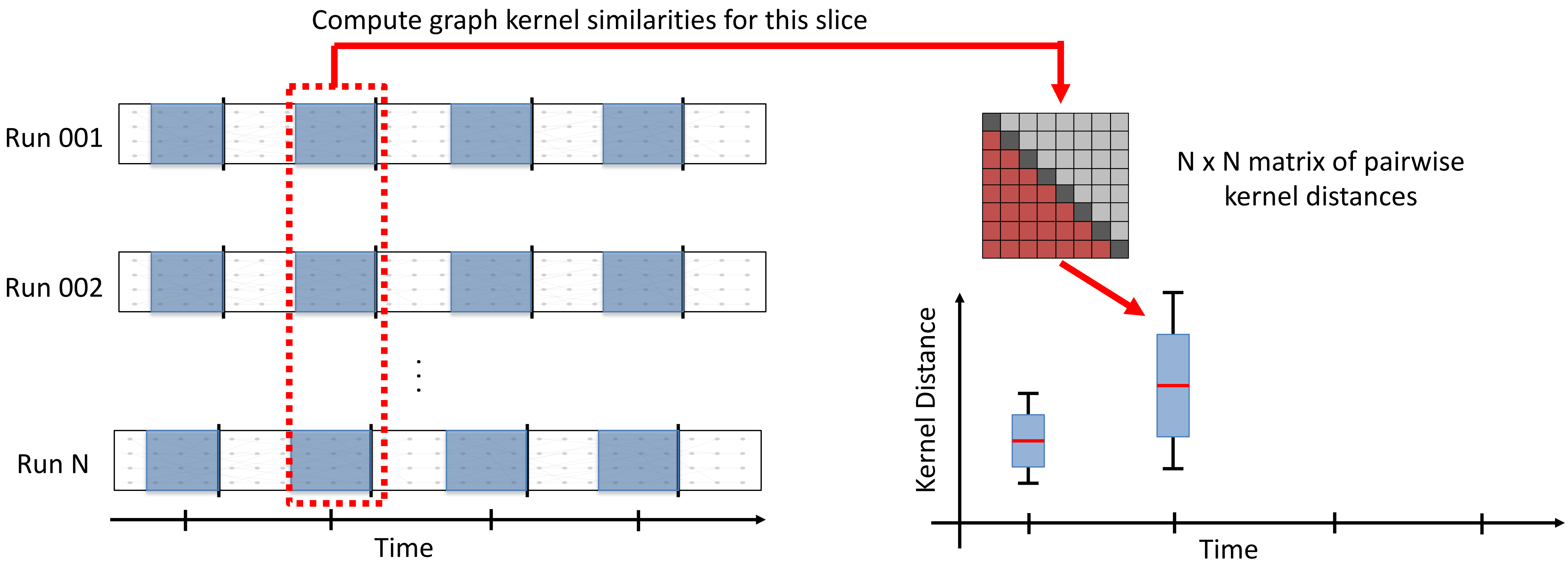
Event Graph Slicing



Distributions of Kernel Distances



Kernel Distance Trends Over Time



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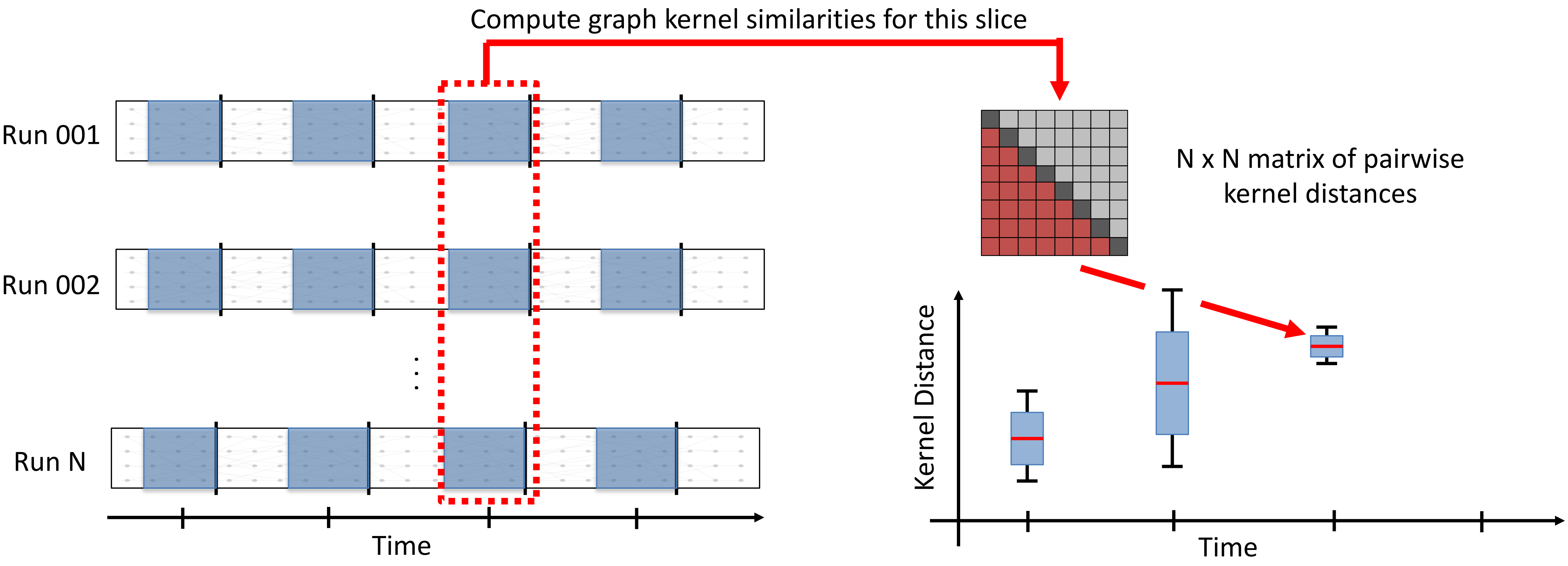

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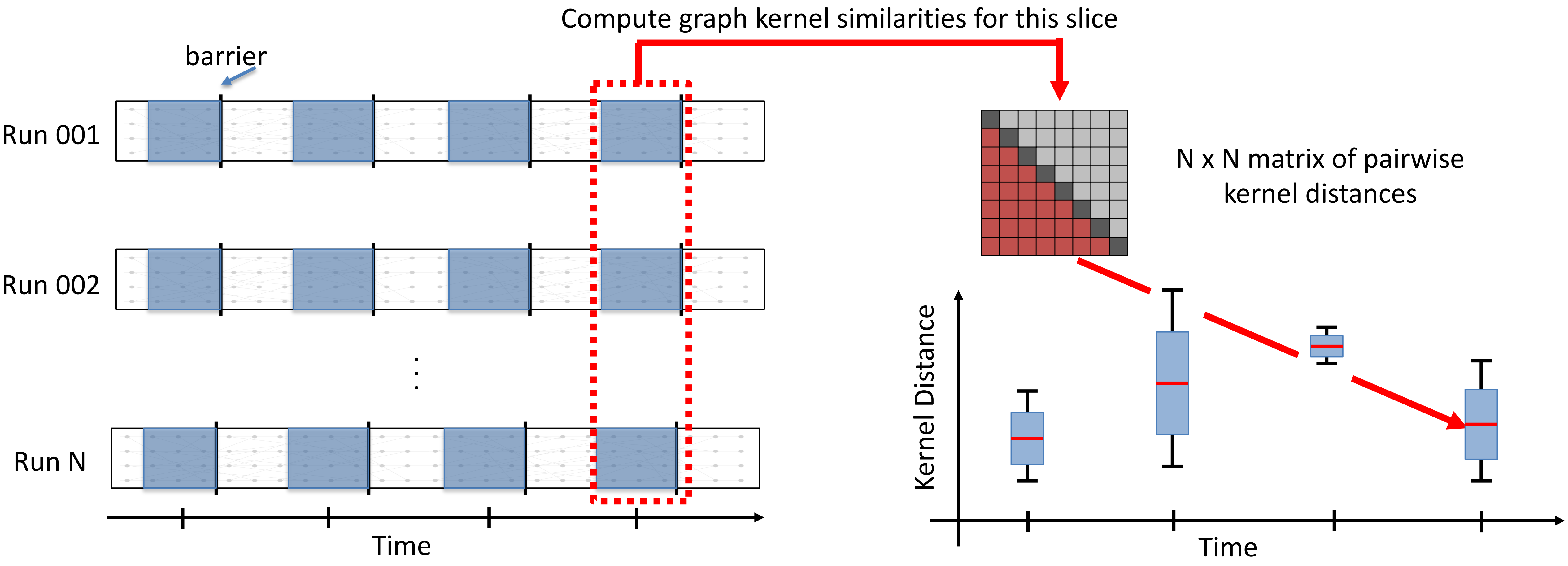
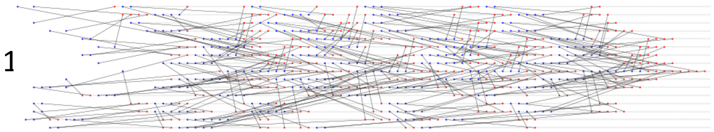
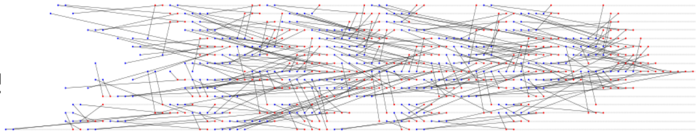
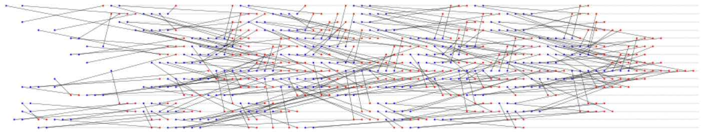


Linking Observed Non-Determinism to Root Causes

Run 1


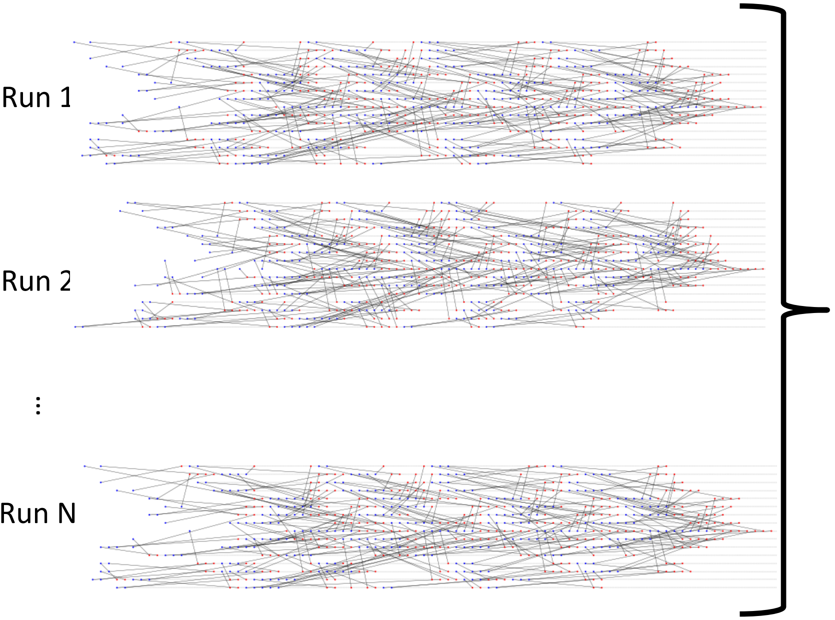
Run 2


⋮

Run N


A set of N event graphs
modeling N runs of a
non-deterministic application

Linking Observed Non-Determinism to Root Causes



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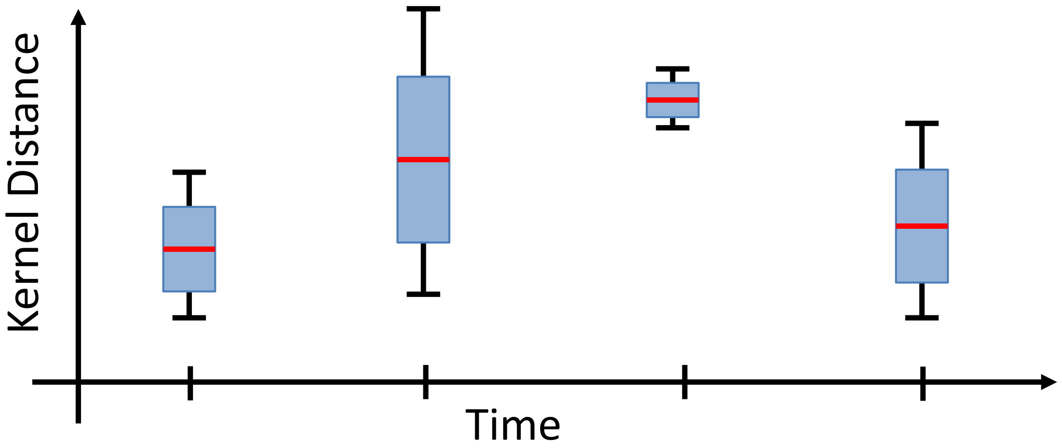
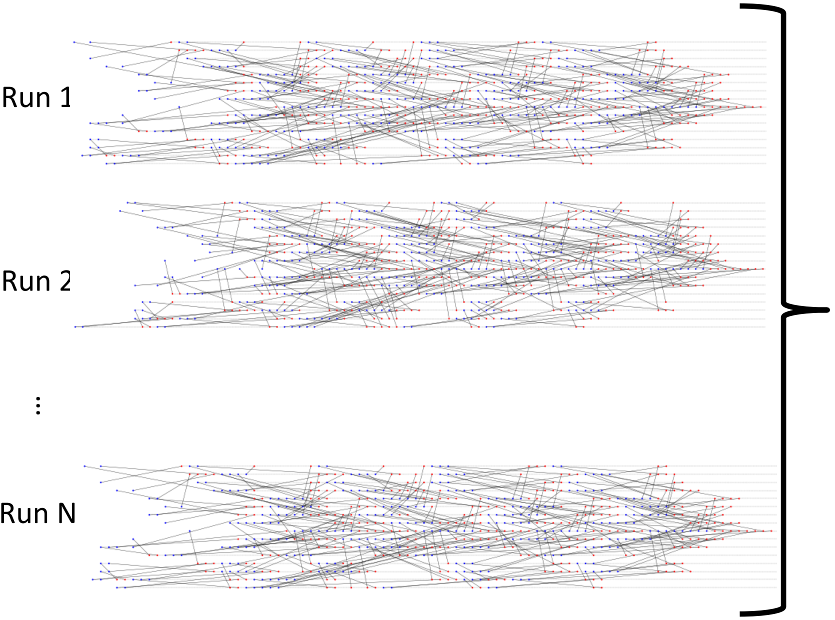


A time-series of distributions of graph kernel distances
between corresponding subgraphs
from pairs of runs

Linking Observed Non-Determinism to Root Causes



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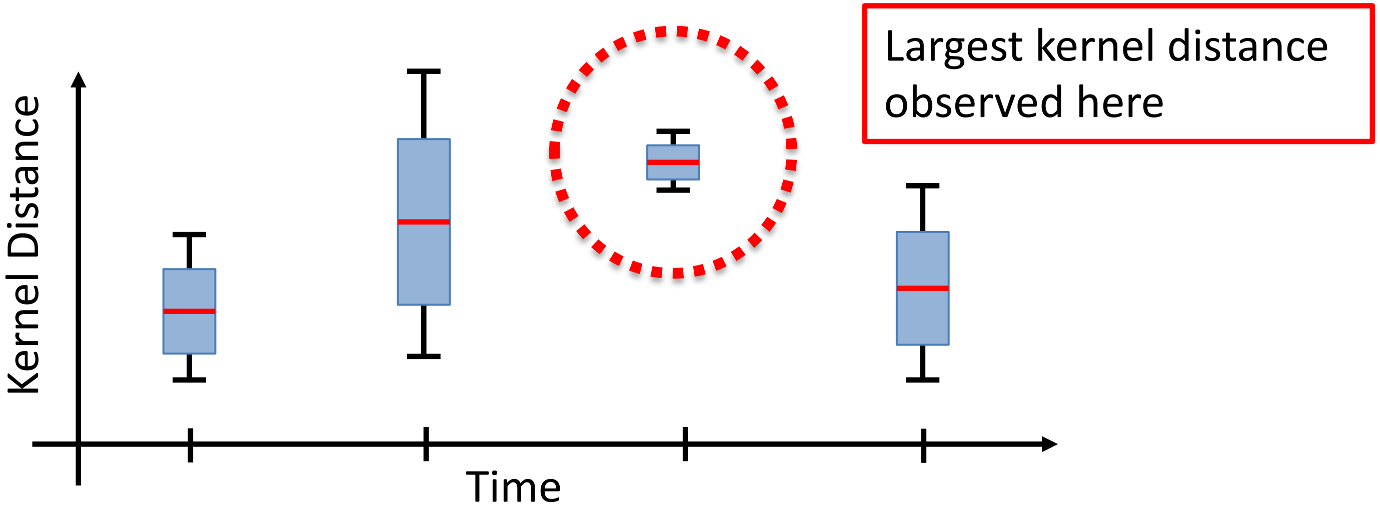

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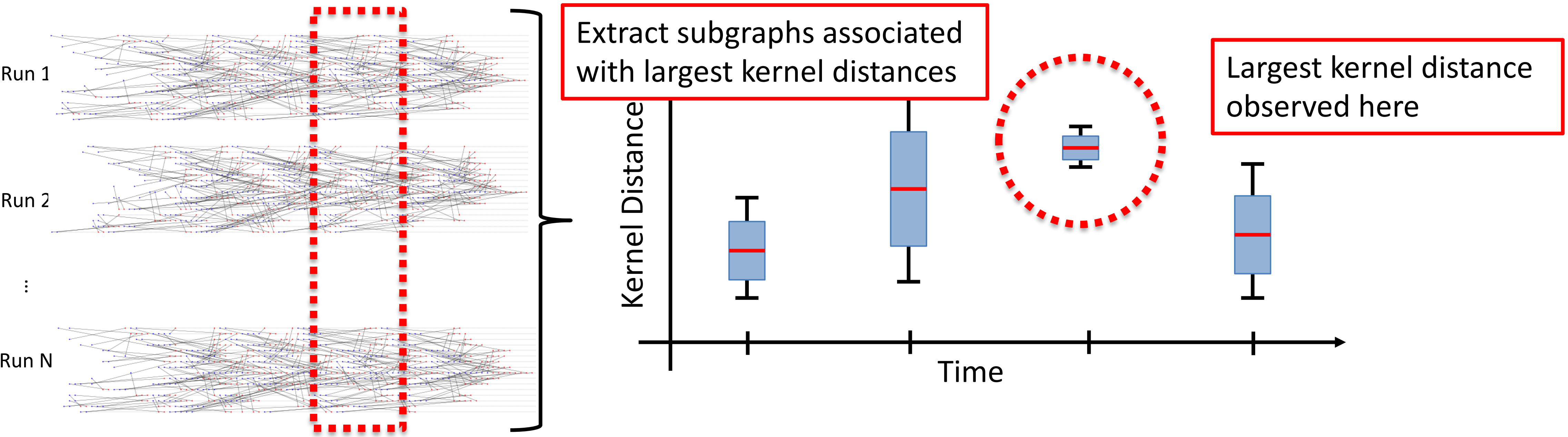
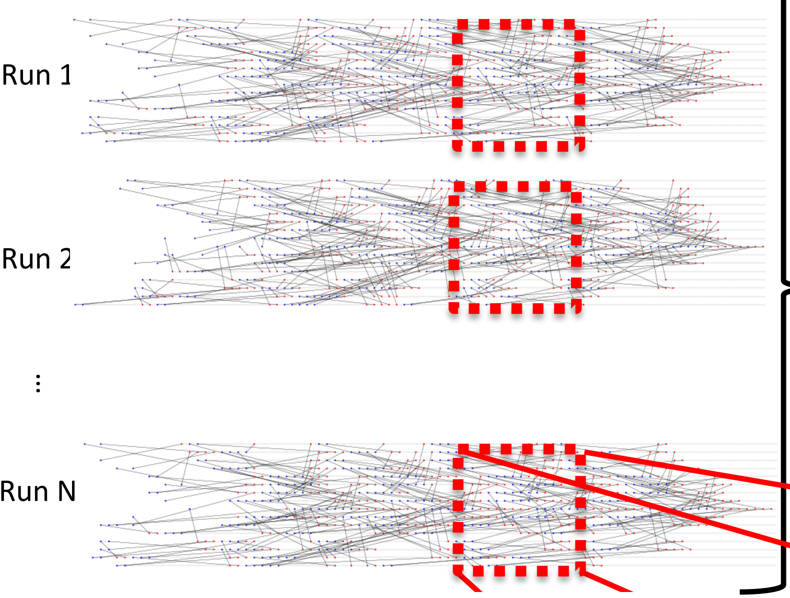


A set of N event graphs modeling N runs of a non-deterministic application

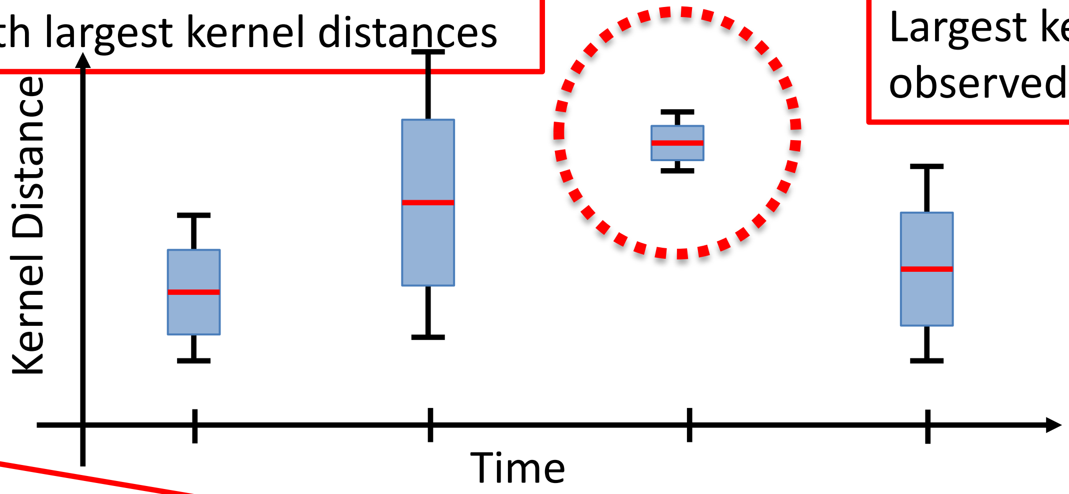
A time-series of distributions of graph kernel distances between corresponding subgraphs from pairs of runs

Linking Observed Non-Determinism to Root Causes



A set of N event graphs modeling N runs of a non-deterministic application

Extract subgraphs associated with largest kernel distances

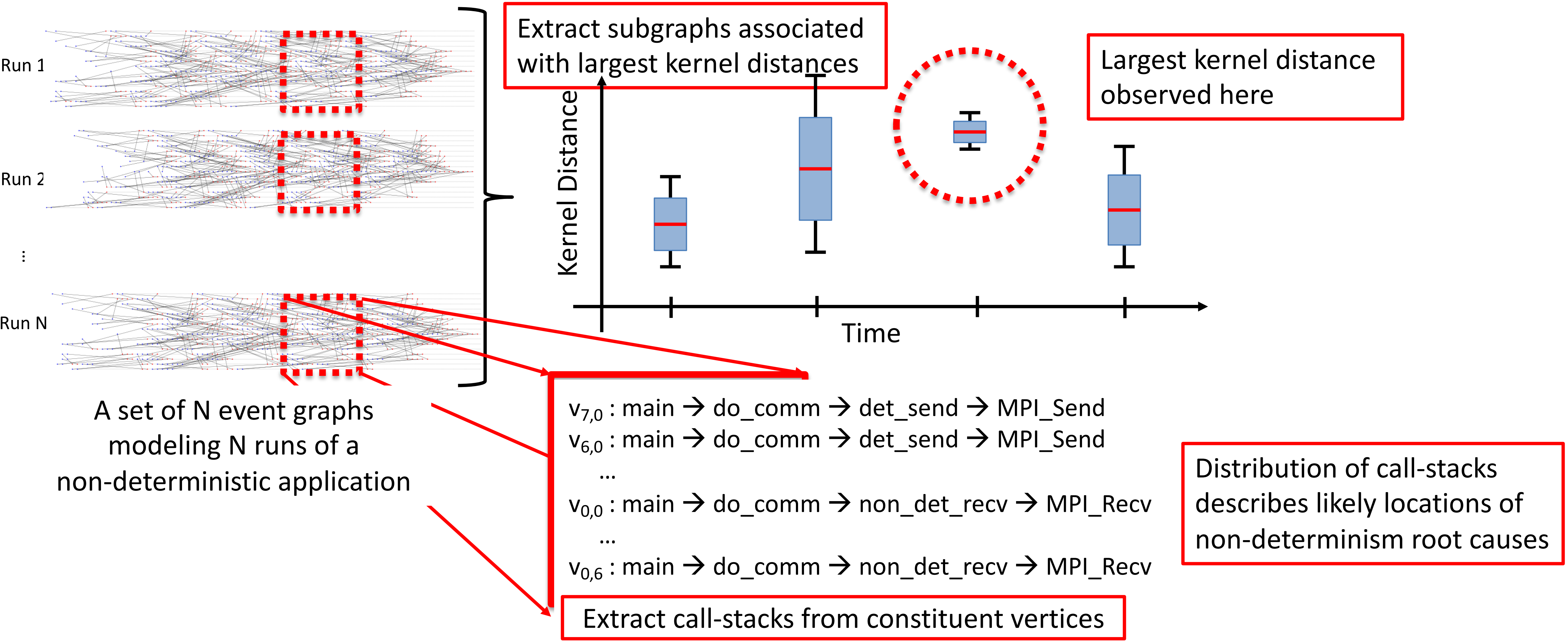


Largest kernel distance observed here

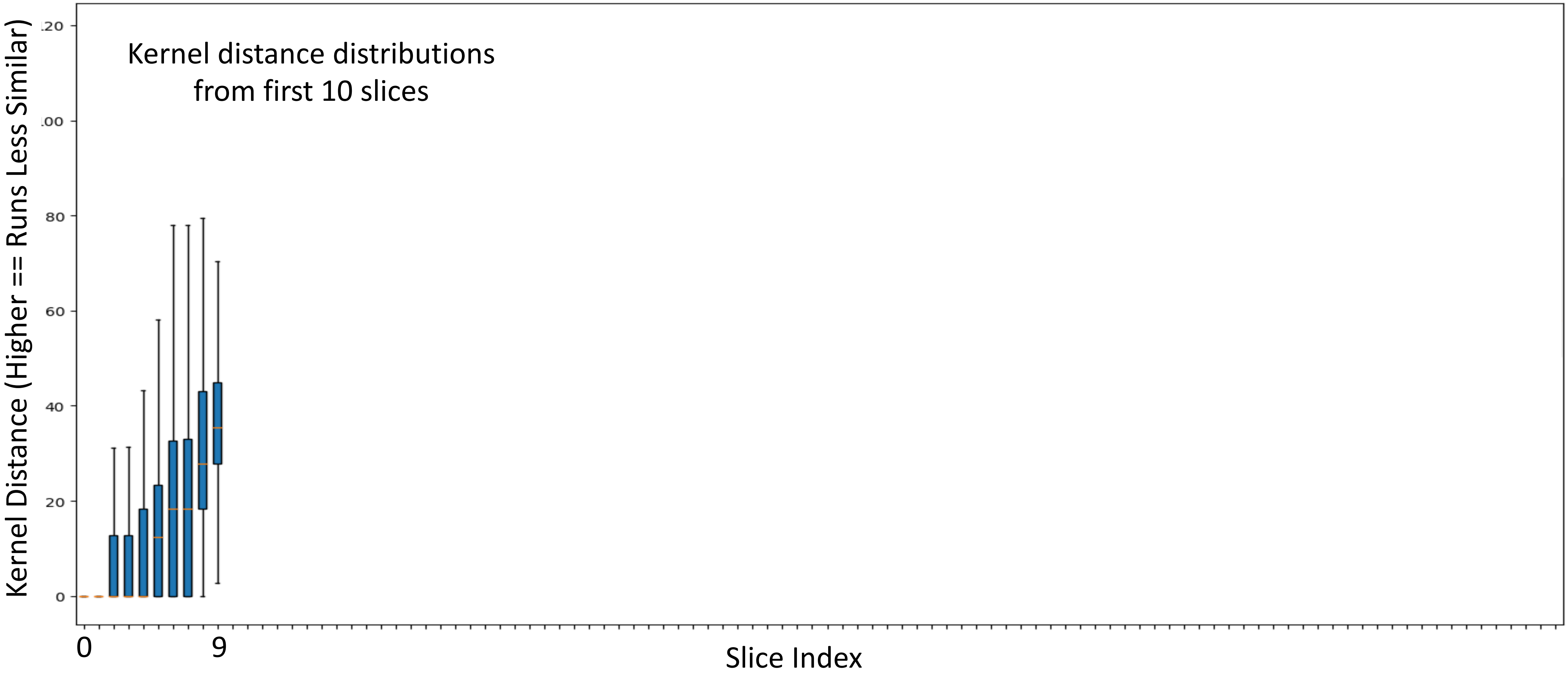
$v_{7,0}$: main → do_comm → det_send → MPI_Send
$v_{6,0}$: main → do_comm → det_send → MPI_Send
…
$v_{0,0}$: main → do_comm → non_det_recv → MPI_Recv
…
$v_{0,6}$: main → do_comm → non_det_recv → MPI_Recv

Extract call-stacks from constituent vertices

Linking Observed Non-Determinism to Root Causes



Kernel Distance Time Series for miniAMR



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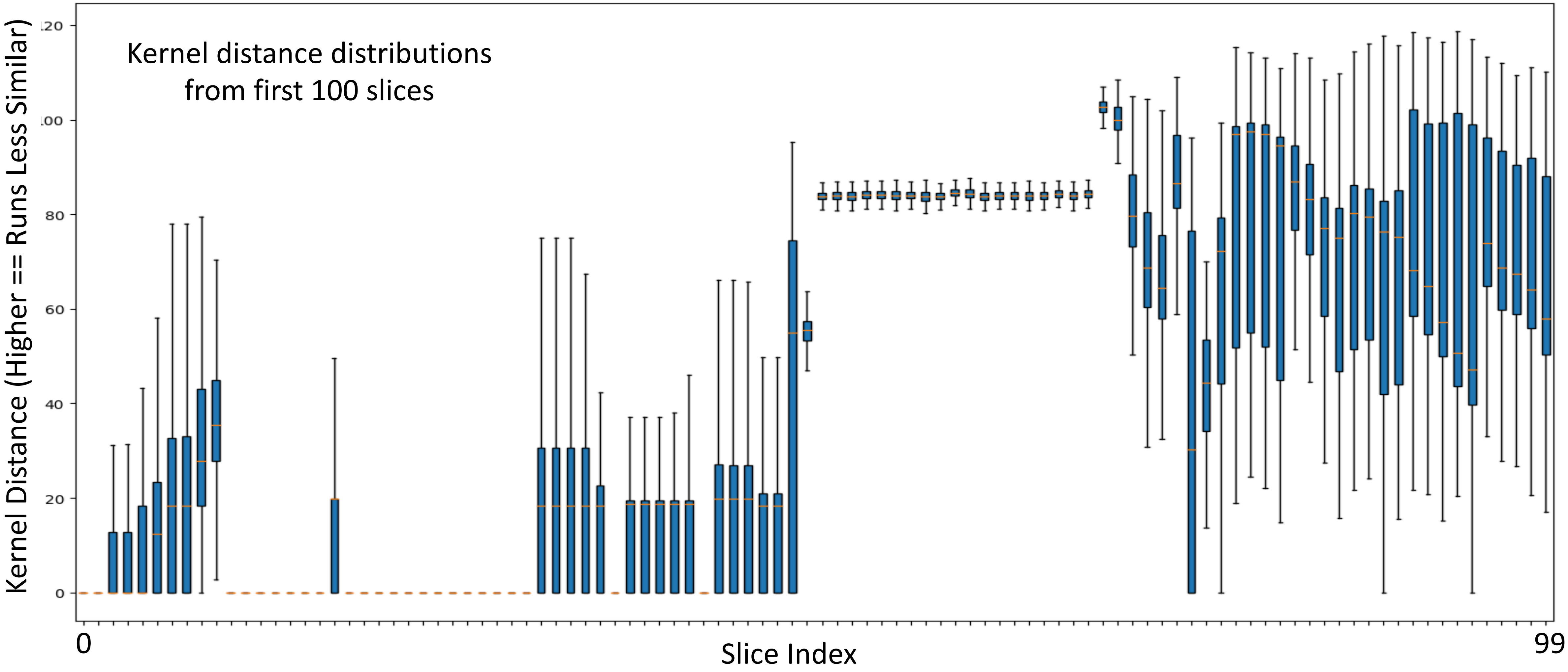

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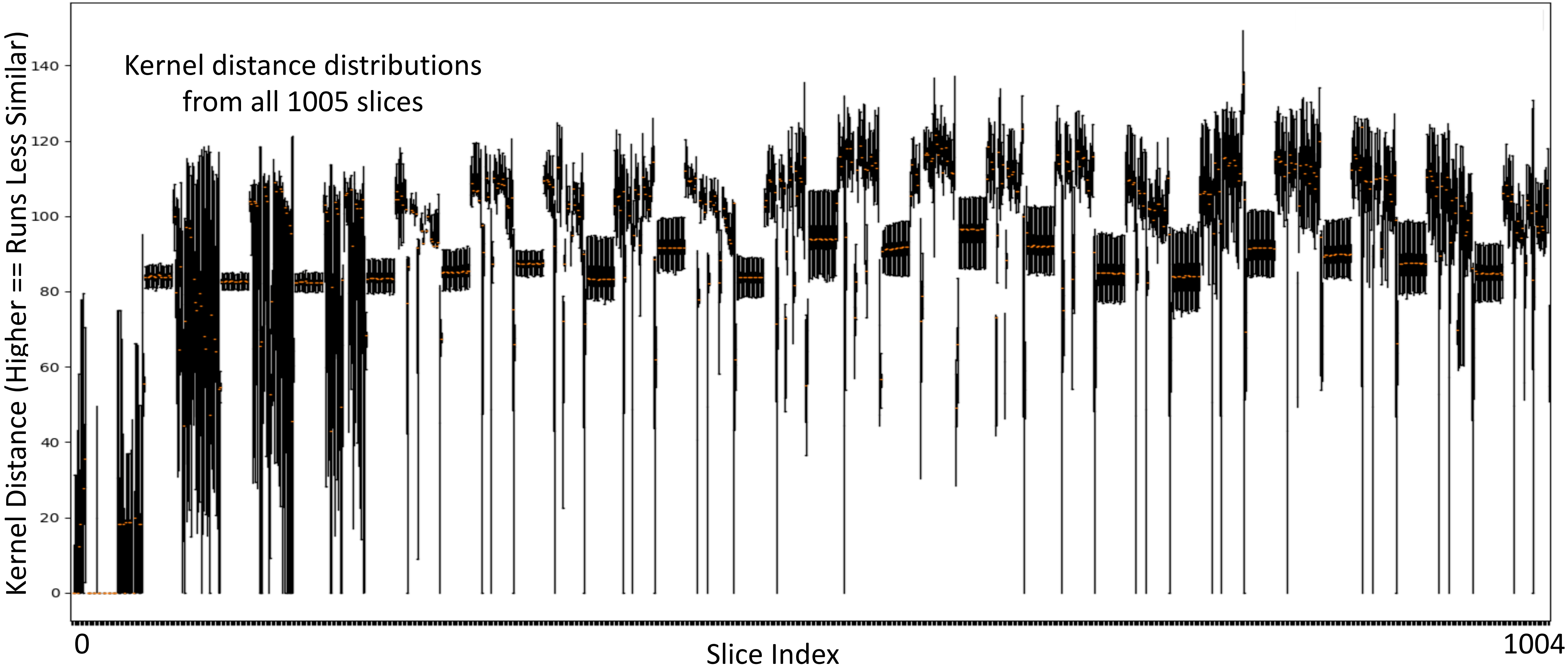
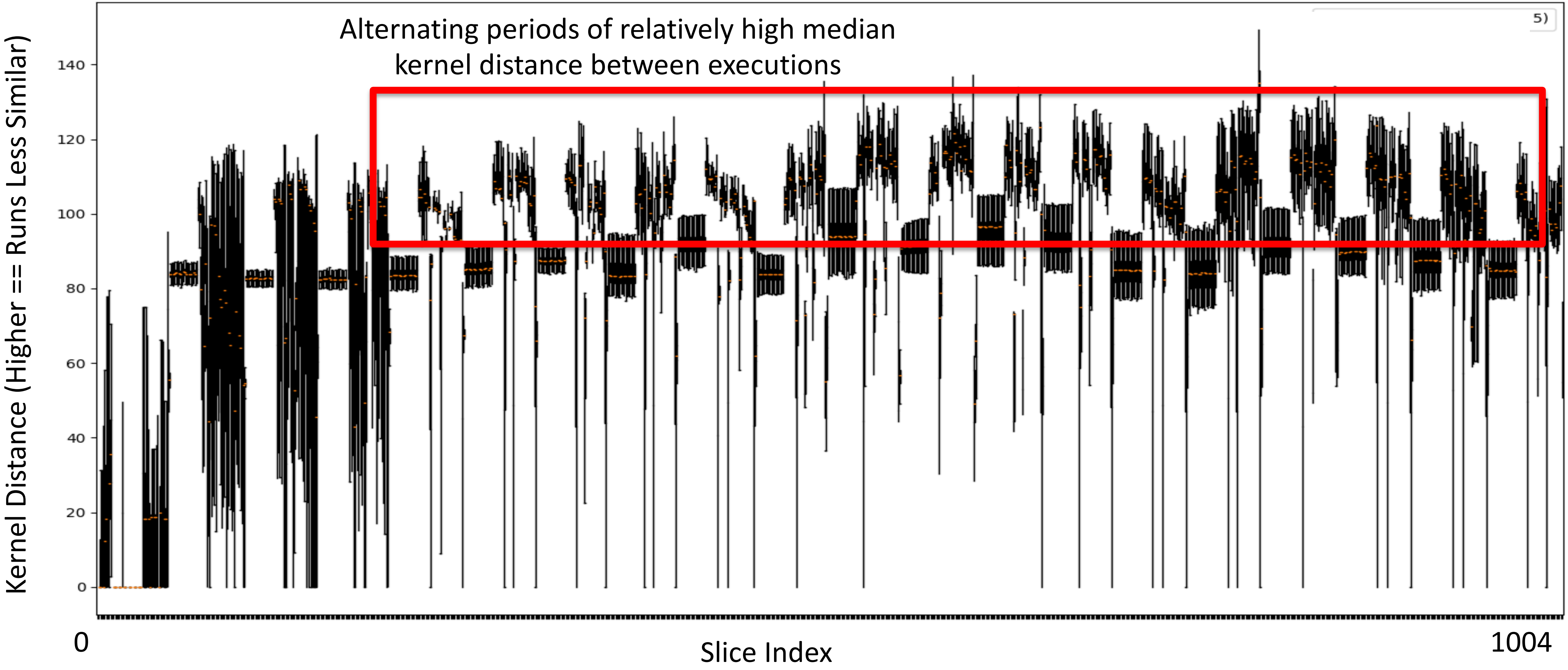


Identifying Anomalous Slices



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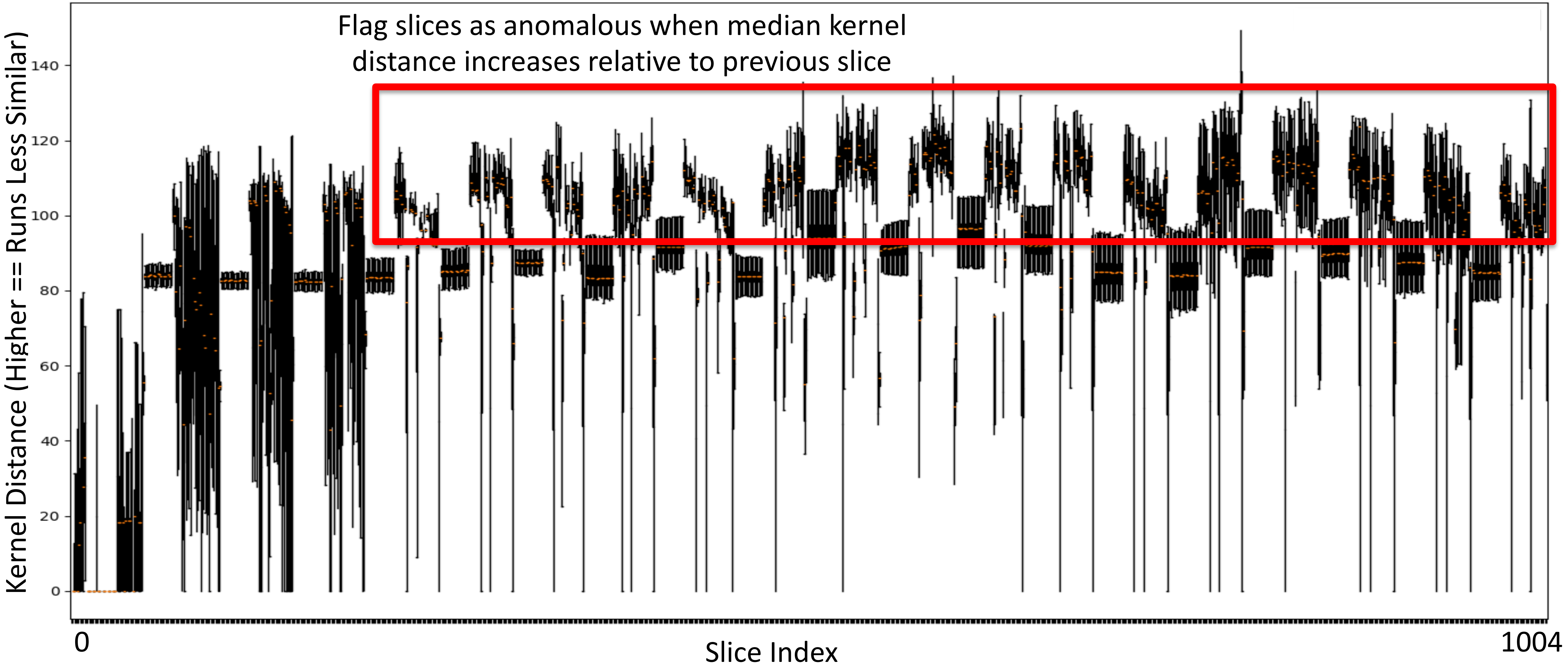
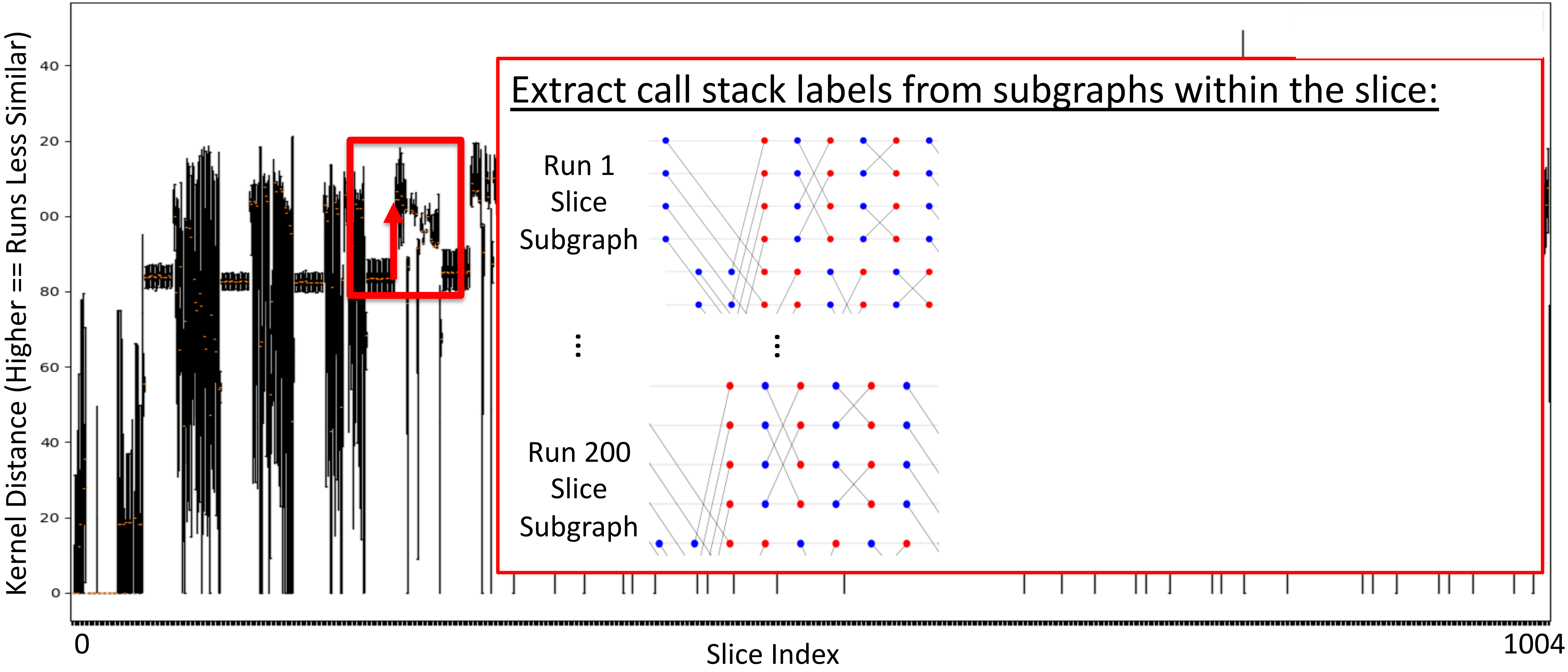


Linking to Potential Root Causes



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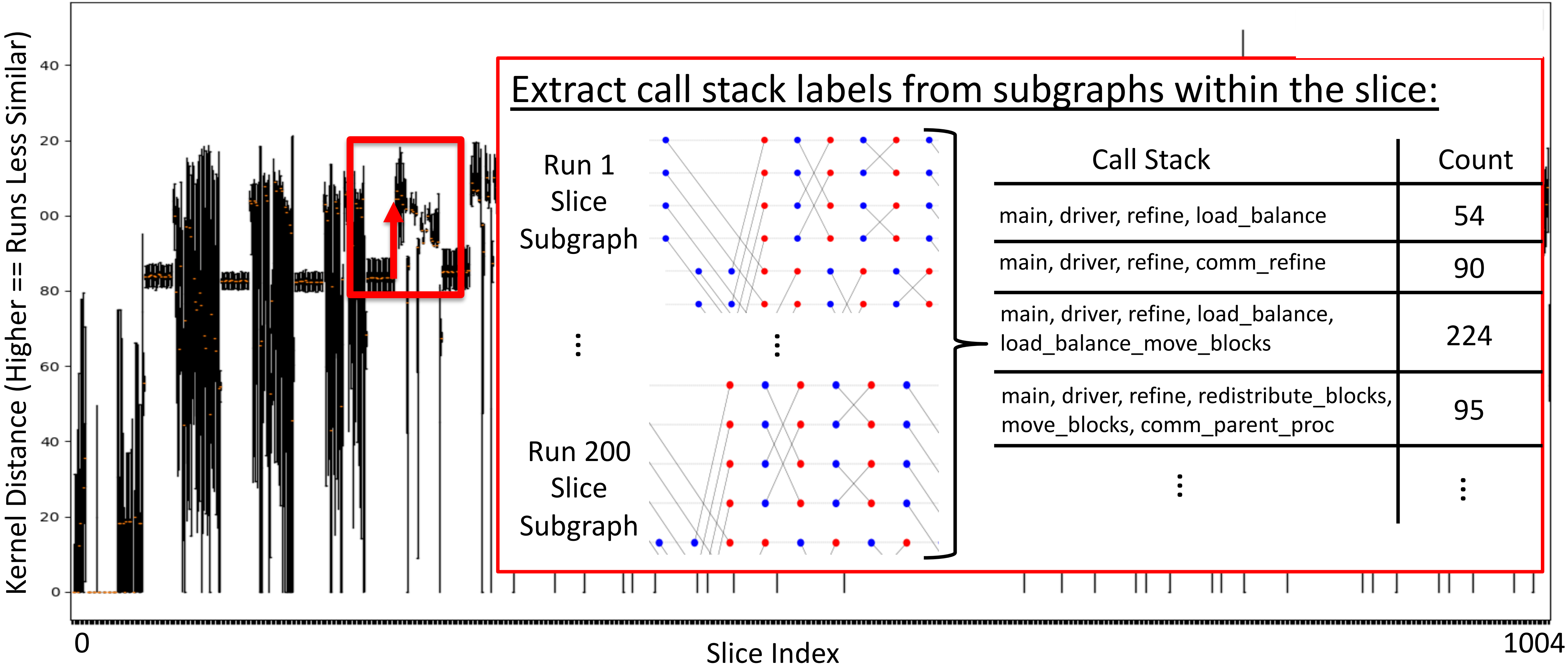
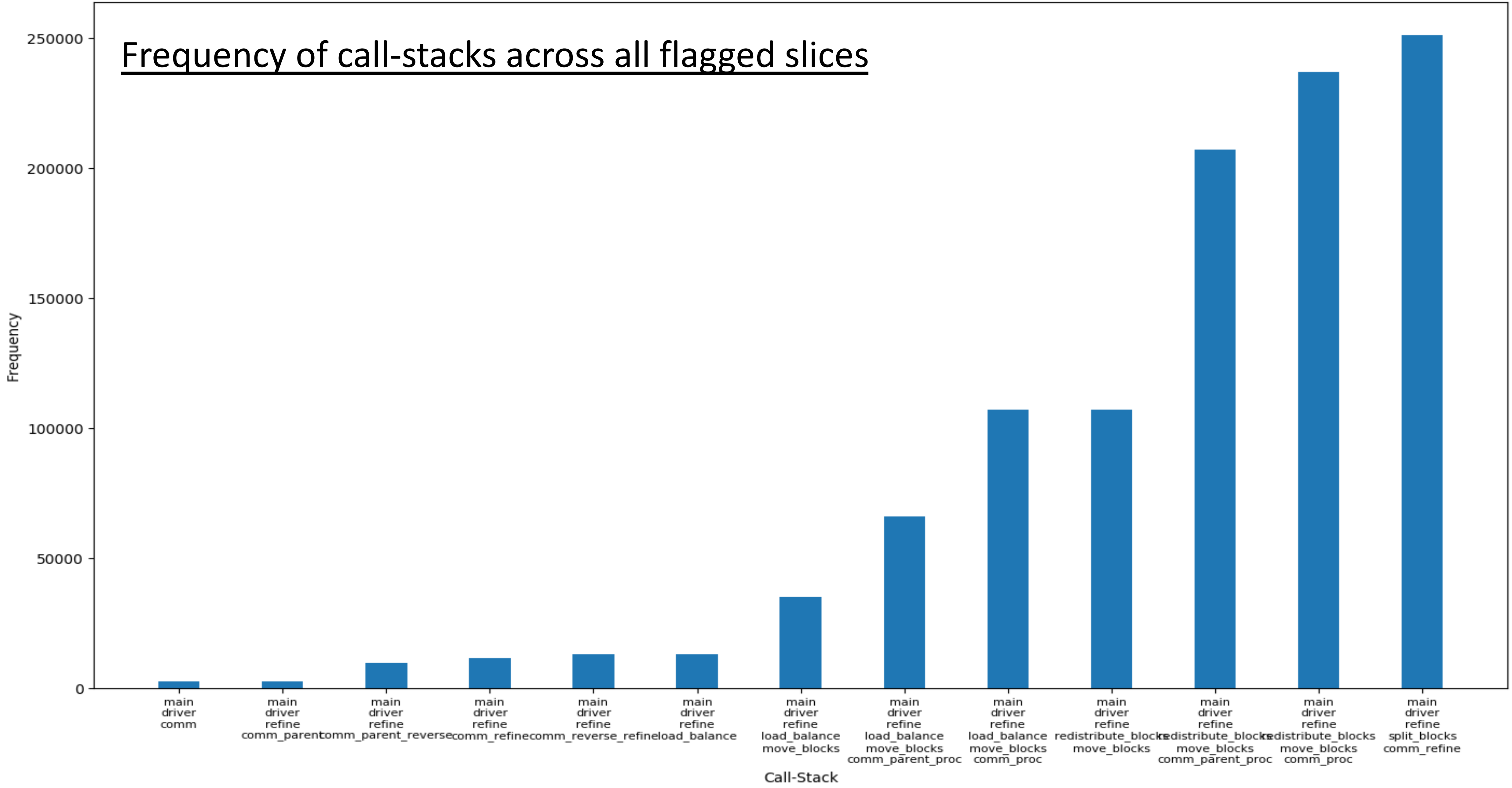


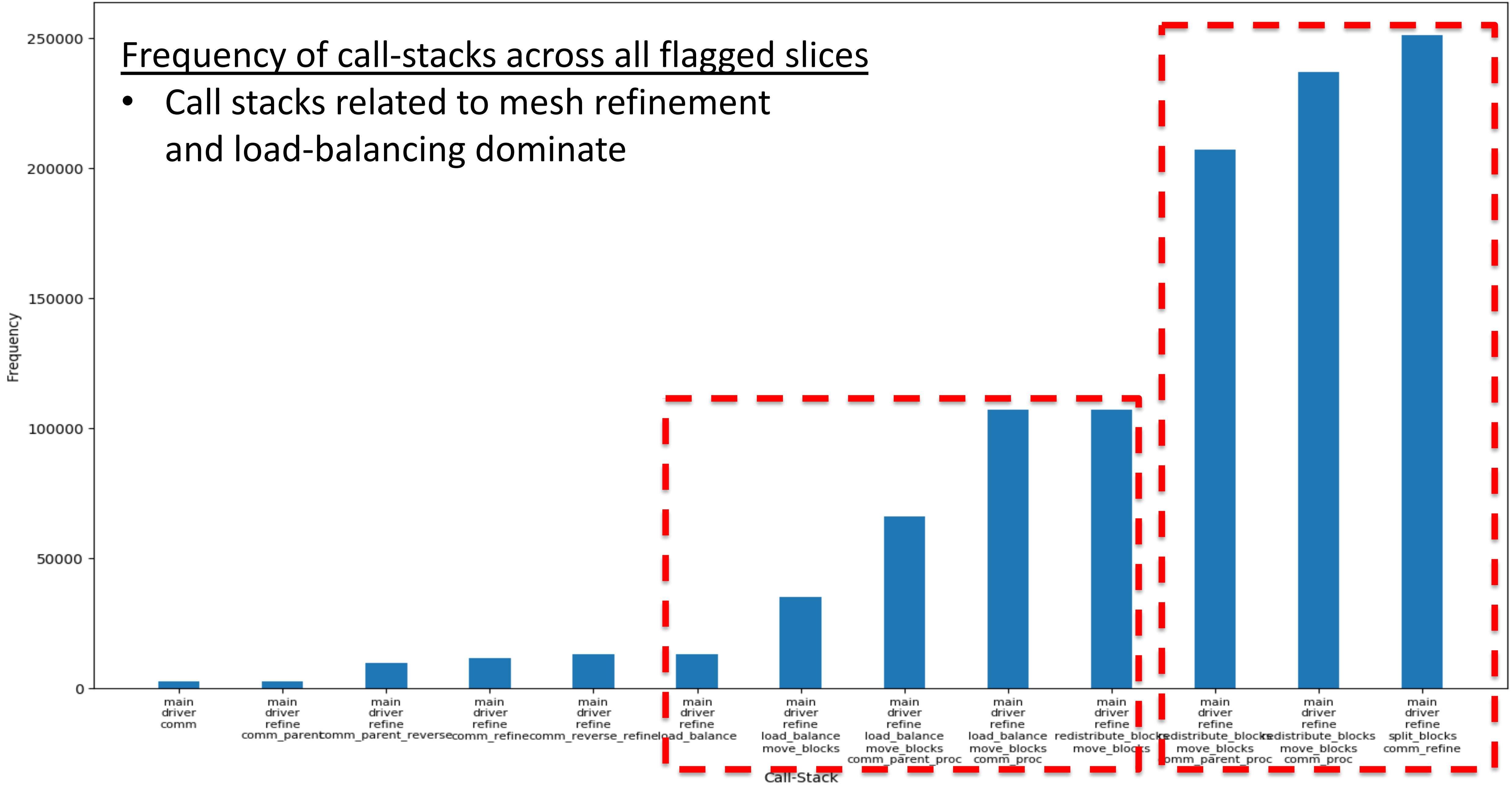
Call Stack	Count
main, driver, refine, load_balance	54
main, driver, refine, comm_refine	90
main, driver, refine, load_balance, load_balance_move_blocks	224
main, driver, refine, redistribute_blocks, move_blocks, comm_parent_proc	95
⋮	⋮



Frequency of call-stacks across all flagged slices
Frequency
250000
200000
150000
100000
50000
0
main driver comm
main driver refine comm_parent
main driver refine comm_parent_reverse
main driver refine comm_refine
main driver refine comm_reverse_refine
main driver refine load_balance
main driver refine load_balance move_blocks
main driver refine load_balance move_blocks comm_parent_proc
main driver refine load_balance move_blocks comm_proc
main driver refine redistribute_blocks move_blocks
main driver refine redistribute_blocks move_blocks comm_parent_proc
main driver refine redistribute_blocks move_blocks comm_proc
main driver refine split_blocks comm_refine
Call-Stack

Frequency of call-stacks across all flagged slices

- Call stacks related to mesh refinement and load-balancing dominate



Conclusion

- Our workflow identifies potential root causes of non-determinism in HPC applications by:
  - Building event graph models of executions
  - Quantifying trends in non-determinism via graph kernel distance
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  - Representative mini-app (miniAMR)

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- Demonstrated viability against:
  - Isolated communication patterns (CORAL-2 AMG)
  - Representative mini-app (miniAMR)
- Future Work:
  - Target full-fledged production AMR applications (e.g., Enzo)

Questions?

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