

Tutorial: Detecting Performance Variance on Large-Scale Heterogeneous Systems



Xin You

Beihang University

Hands-on Tutorial @ CLUSTER25



北京航空航天大学
BEIHANG UNIVERSITY

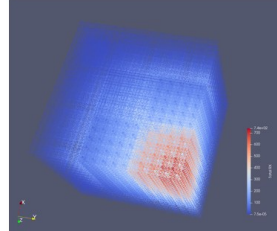
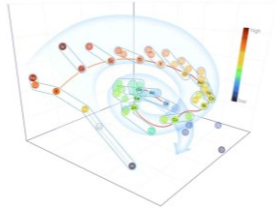
Outline

- Introduction
- Design Overview
- Detecting Performance Variance & Implementation
- Evaluation
- Hand-on Tutorial

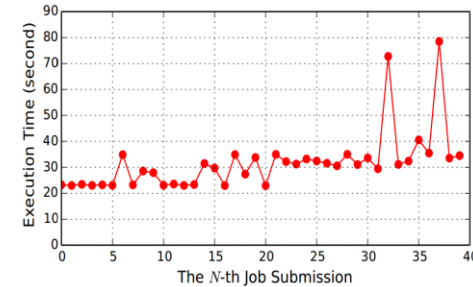
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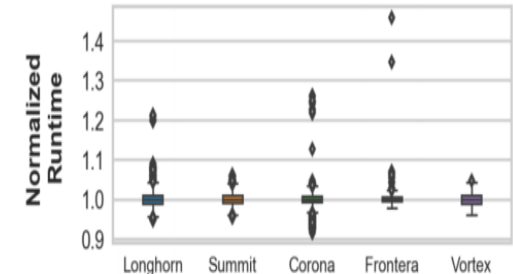
Large-Scale Heterogenous System



Various production and scientific applications

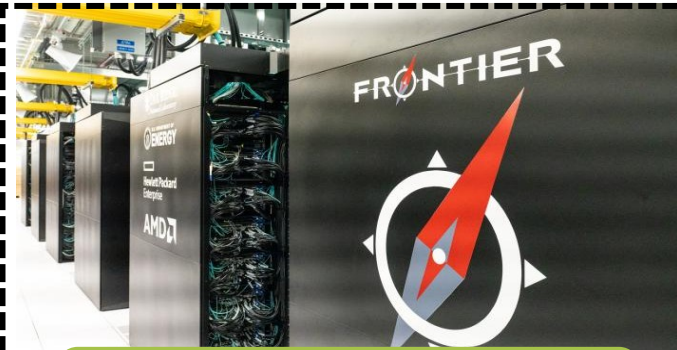


Performance variance in homogeneous systems (Zheng et.al., PPOPP22)



Performance variance in heterogenous systems (Sinha et.al., SC22)

Computational support



Frontier: >37K GPUs
X86 + GPU (#1@2024.6)



Aurora: >63K GPUs
X86 + GPU (#2@2024.6)

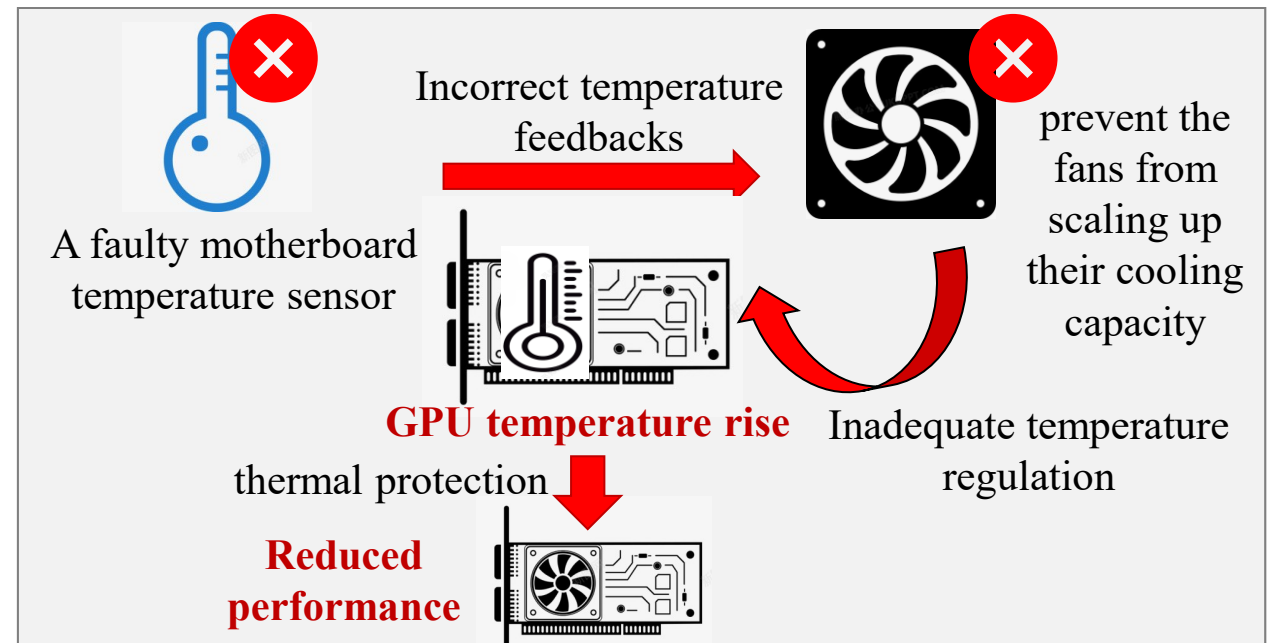
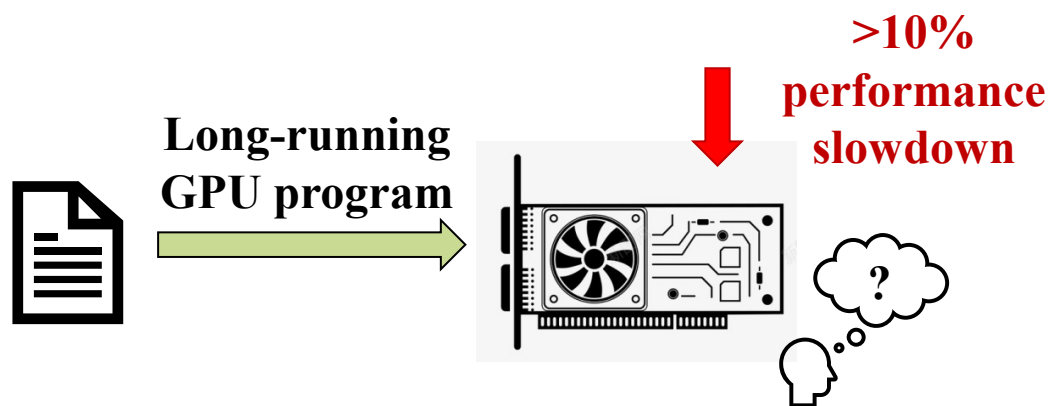
The attainable parallel program performance has **become more and more unstable**

Scale of GPU cluster increases

Performance variance has become one of the nasty pitfalls when running parallel programs on such large-scale heterogeneous systems.

Diagnosing Performance Variance: Real Case

- Performance variance often suffers from its **spontaneity, unpredictability, and the diversity** of root causes
 - making it **exceedingly difficult** to detect and pinpoint the underlying reasons for potential performance variance during program execution.

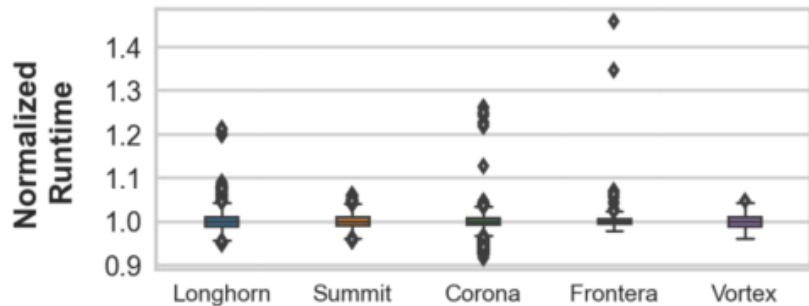


Pinpointing the precise root causes of such performance variances remains a formidable task for both developers and system maintainers

Challenges in Existing Approaches

Microbenchmark based

- The most widely adopted approaches to discover and diagnose the source of the performance variance
- Require the same well-formed workloads running on different computation nodes for performance variance detection



Uncovered performance variances in large-scale heterogeneous systems caused by GPU hardware variances.

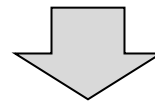


- ❑ Based on **long-term data collection** using specific micro-benchmarks
- ❑ Cannot capture and identify potential performance variances **during program execution**

Challenges in Existing Approaches

Microbenchmark based

- The most widely adopted approaches to discover and diagnose the source of the performance variance
- Require the same well-formed workloads running on different computation nodes for performance variance detection



detecting and reasoning performance variance
within a single parallel execution.

Fixed workload based

- Identified several fixed-workload code snippets that can be treated as probes for performance variance detection of homogeneous systems
 - Based on observations that codes with similar workload should result in similar performance with the same hardware and software specifications

Challenges in Existing Approaches



- ✓ Address performance variances and root cause analysis to some extent in large-scale homogeneous systems



- ❑ Fail to track **asynchronous** communications
- ❑ They are not directly applicable to **heterogeneous systems**
- ❑ GPU diagnosis tools (e.g., DrGPU) incurs **high overhead** to pinpoint the causes of poor performance on GPU-based programs

Still lack an effective tool to detect performance variance for **large-scale heterogeneous systems**

Fixed workload based

- Identified several fixed-workload code snippets that can be treated as probes for performance variance detection of homogeneous systems
 - Based on observations that codes with similar workload should result in similar performance with the same hardware and software specifications

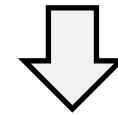
Challenges in Existing Approaches



- ✓ Address performance variances and root cause analysis to some extent in large-scale homogeneous systems



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Key challenges:

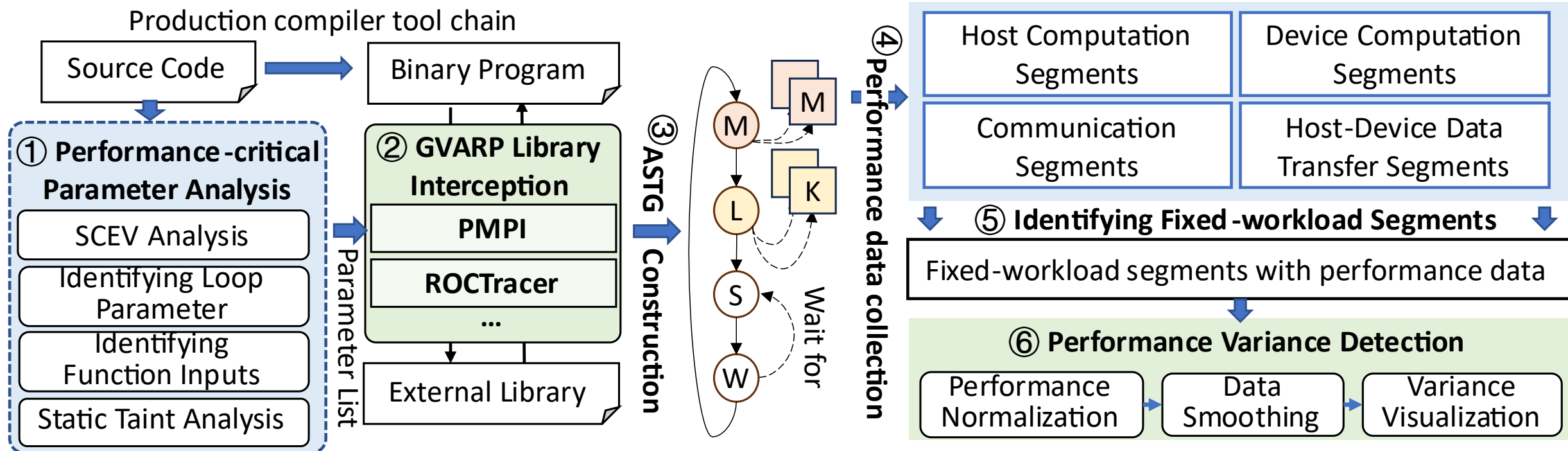
- 1) *How to identify **fixed-workload** probes within parallel programs for **heterogeneous systems**?*
 - including kernel, CPU-GPU data transfer, sync/async communications, etc.
- 2) *How to **collect performance data** for performance variance detection **at a low cost**?*
 - high overhead may mislead the identification of performance variances

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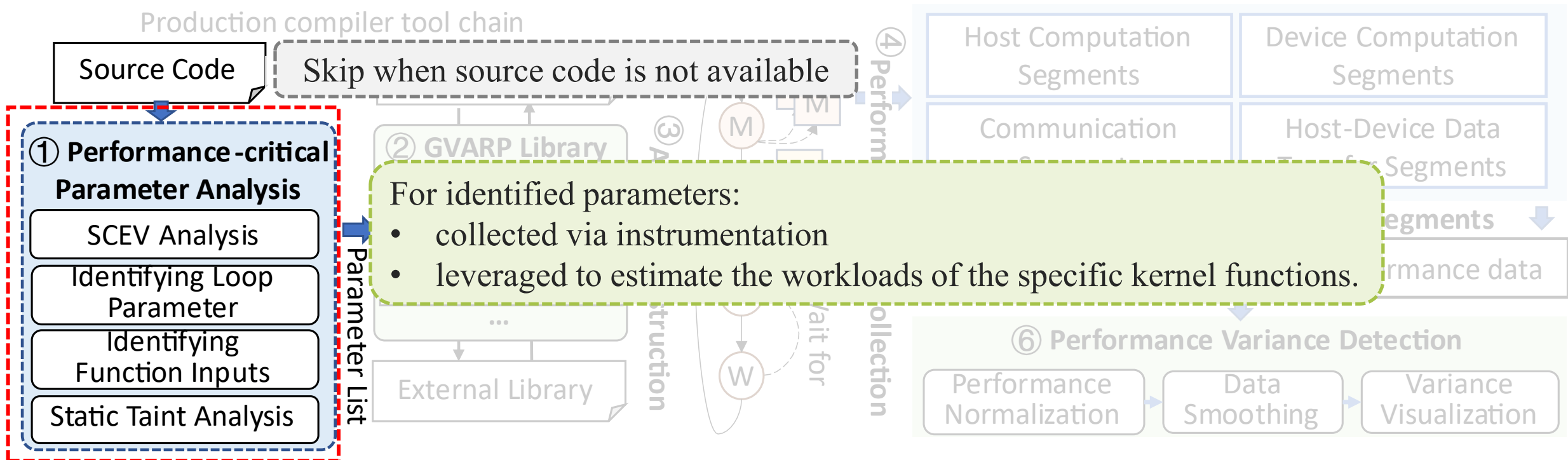
Design Overview

- We propose GVARP, a performance variance detection tool for large-scale heterogeneous systems.
- No mandatory need for customized compiler chains or recompilation



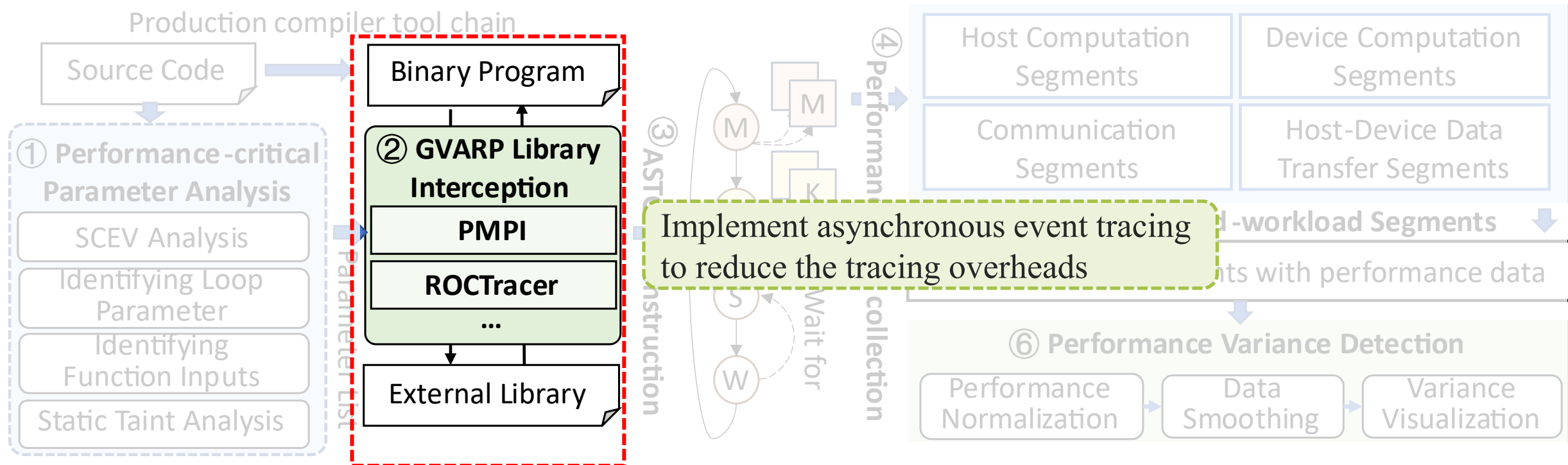
Design Overview

- We propose GVARP, a performance variance detection tool for large-scale heterogeneous systems.
 - 1) Analyzes the source code to identify all accelerated kernel functions on GPU and identify **the performance-critical parameters** via static taint analysis



Design Overview

- We propose GVARP, a performance variance detection tool for large-scale heterogeneous systems.
- 2) GVARP divides the execution of a parallel program into **internal and external program segments** with **external library calls**.



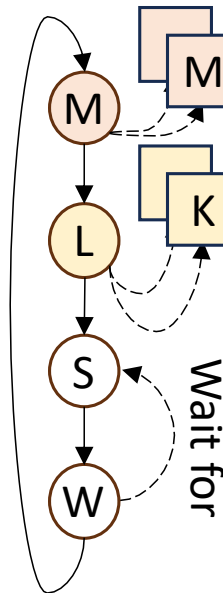
Design Overview

- We propose GVARP, a performance variance detection tool for large-scale heterogeneous systems.
- 3) GVARP constructs **Asynchronous State Transition Graph (ASTG)** from the collected traces to represent the program execution

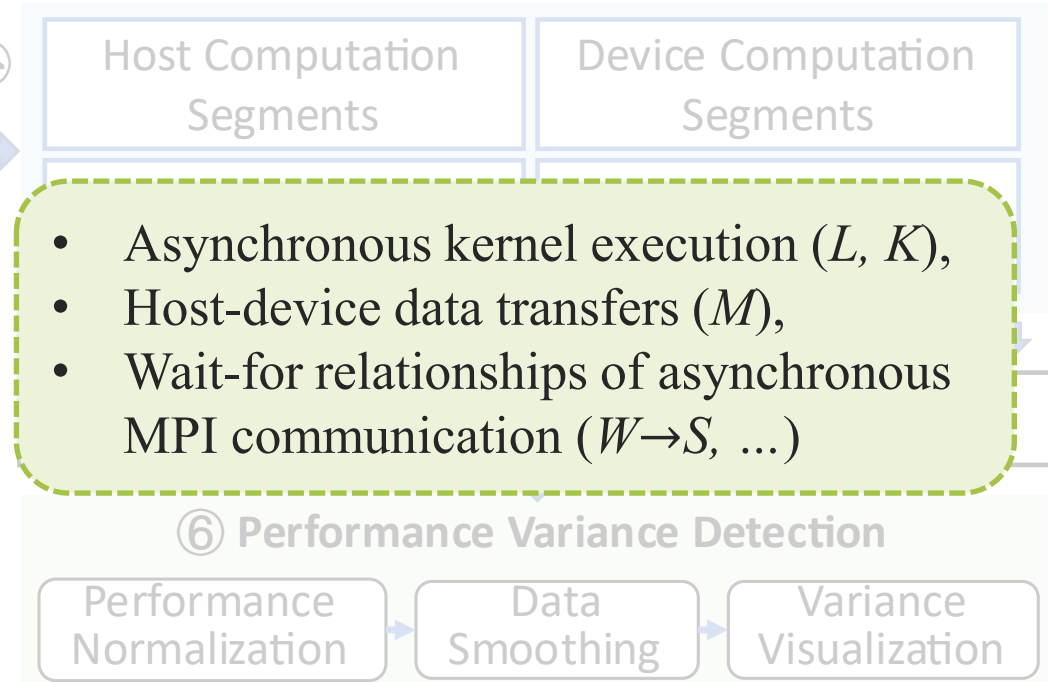
Production compiler tool chain

- Nodes (\bigcirc , e.g., M , L , S , W)
 - host-side external program segments
- Nodes (\square , e.g., M , K)
 - device-side asynchronous events
- Edges (\rightarrow , e.g., $M \rightarrow L$)
 - host-side internal program segments
- Edges (\dashrightarrow , e.g., $W \dashrightarrow S$)
 - asynchronous event annotations

③ ASTG Construction



④ Performance data collection



Design Overview

- We propose GVARP, a performance variance detection tool for large-scale heterogeneous systems.
- 4) **Attributes each program segments with performance data**, including enter and exit timestamps, correlation identifiers, function parameters, and performance counters.

Nodes (\bigcirc , e.g., S , W): Communication Segments

- enter/exit timestamps, $\langle S, D, C, N_{bytes} \rangle$

Nodes (\boxed{K} $\bigcirc L$): Device Computation Segments

- enter/exit timestamps, correlation ID, #threads, #blocks, ...

Nodes (\boxed{M} $\bigcirc M$): Host-Device Data Transfer Segments

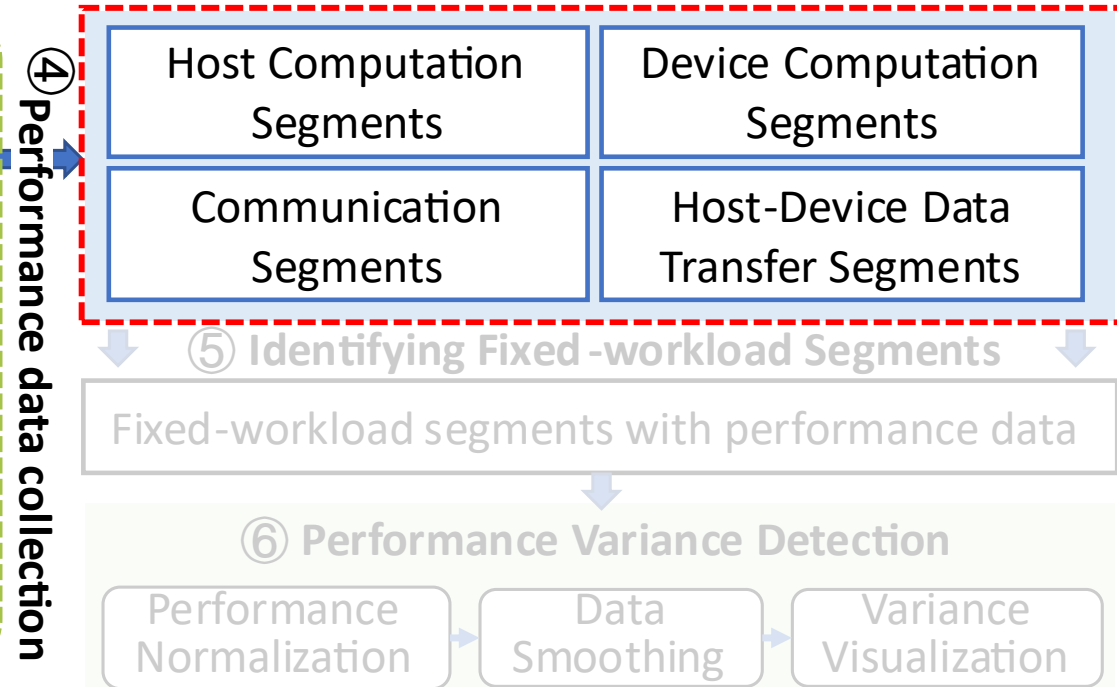
- enter/exit timestamps, correlation ID, $\langle N_{bytes}, kind, S_M \rangle$

Edges (\rightarrow , e.g., $M \rightarrow L$): Host Computation Segments

- enter/exit timestamps, perf. counters (#instruction)

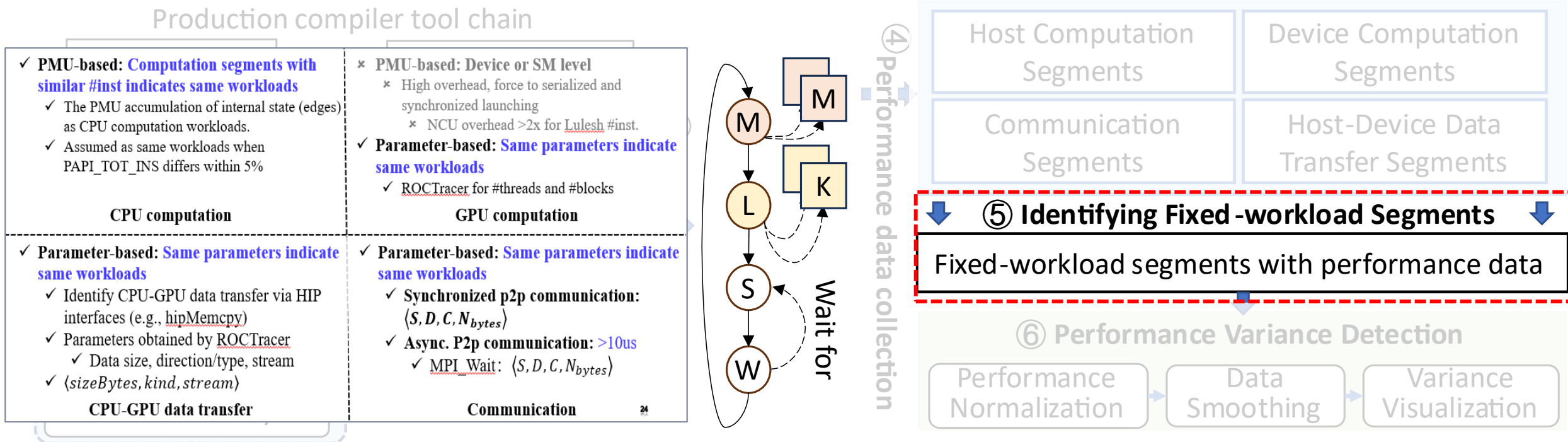
Edges ($\overset{\text{Wait for}}{\dashrightarrow}$, e.g., $W \rightarrow S$): Communication Segments (Async)

- attribute parameters of non-overlapped async. comm.



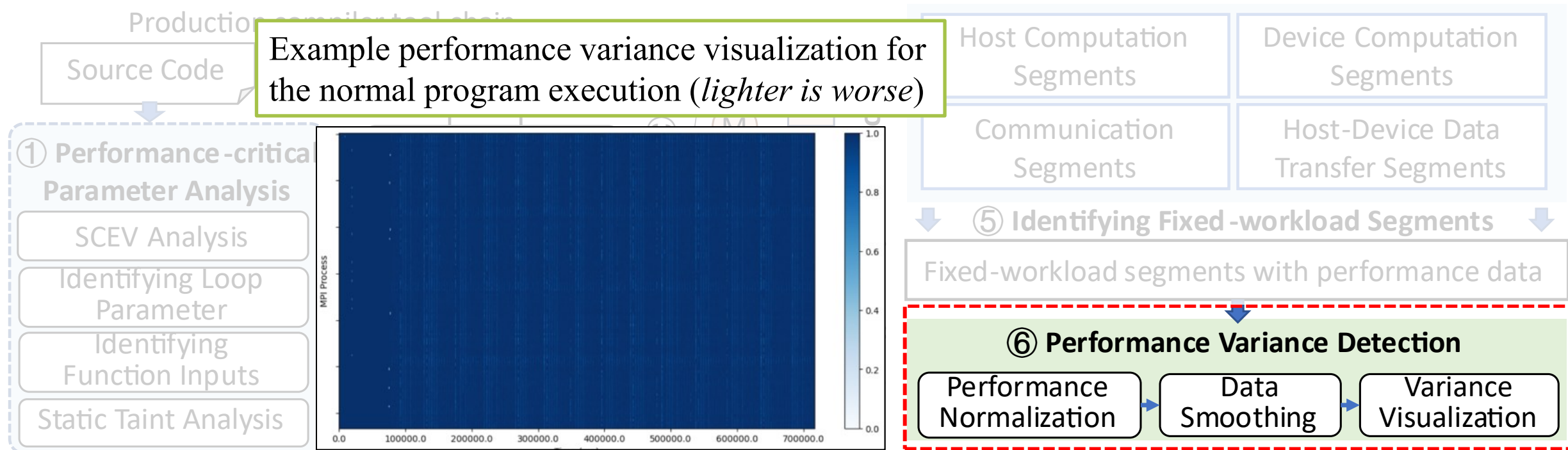
Design Overview

- We propose GVARP, a performance variance detection tool for large-scale heterogeneous systems.
- 5) For each type of program segment, GVARP leverages the **ASTG-based clustering** to **identify fixed-workload segments** for further performance variance detection.



Design Overview

- We propose GVARP, a performance variance detection tool for large-scale heterogeneous systems.
- 6) For each **cluster of fixed-workload segments**, GVARP adopts **performance normalization and data smoothing** for comparable and noiseless variance metrics.

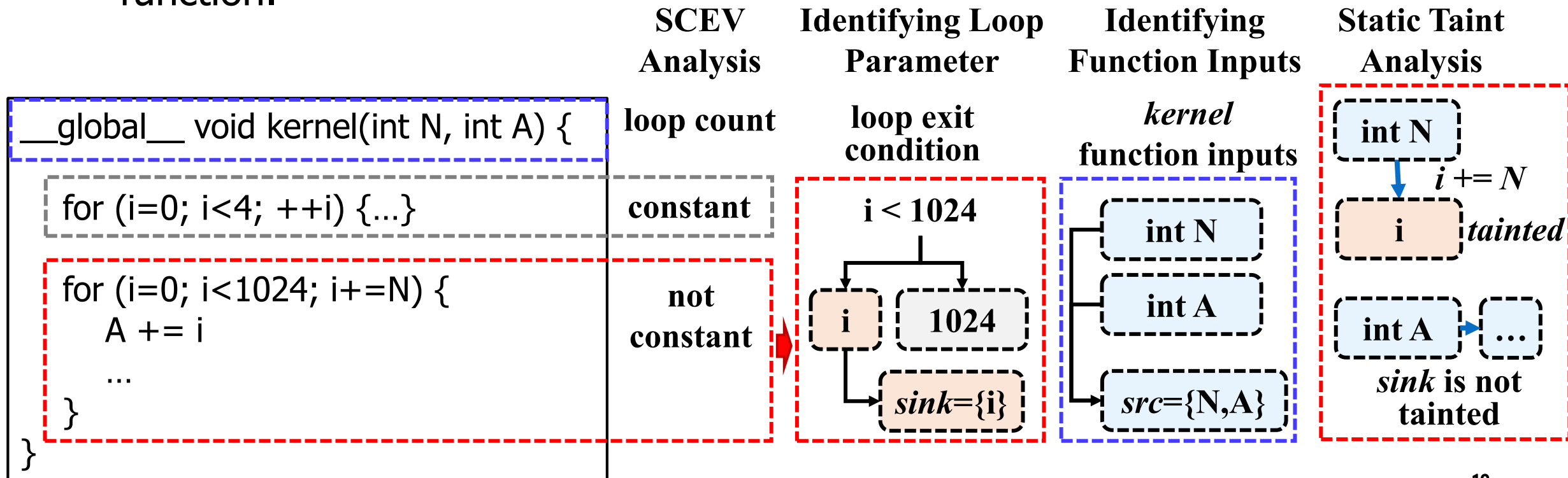


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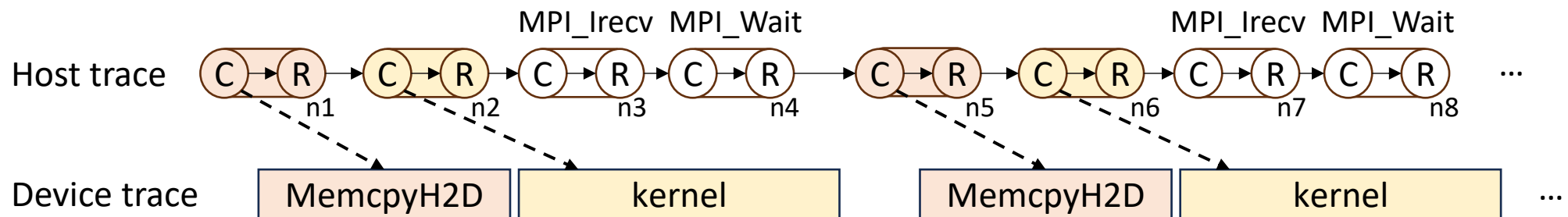
Performance-critical Parameter Analysis

- **Key Idea:** If the value of kernel function parameter can affect the value of loop condition variables, such parameters are *performance-critical*.
 - The performance-critical parameters can affect the loop counts within the function.



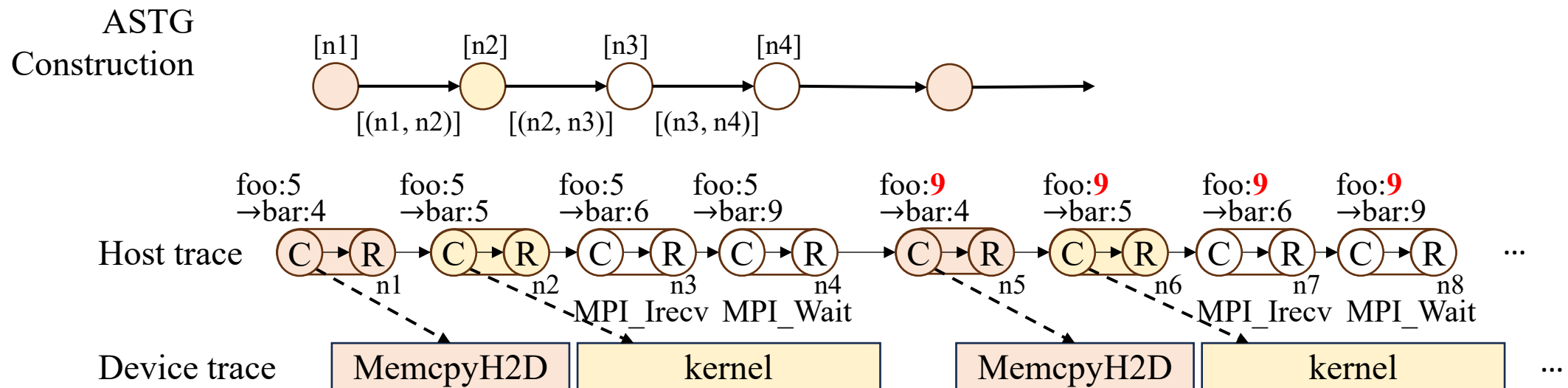
ASTG Construction

- After collecting target program's performance trace, GVARP constructs Asynchronous State Transition Graph (ASTG) based on the collected traces
 - CPU-GPU data transfer (*orange icons*), GPU kernel launch (*yellow icons*) and MPI communication (*white icons*)



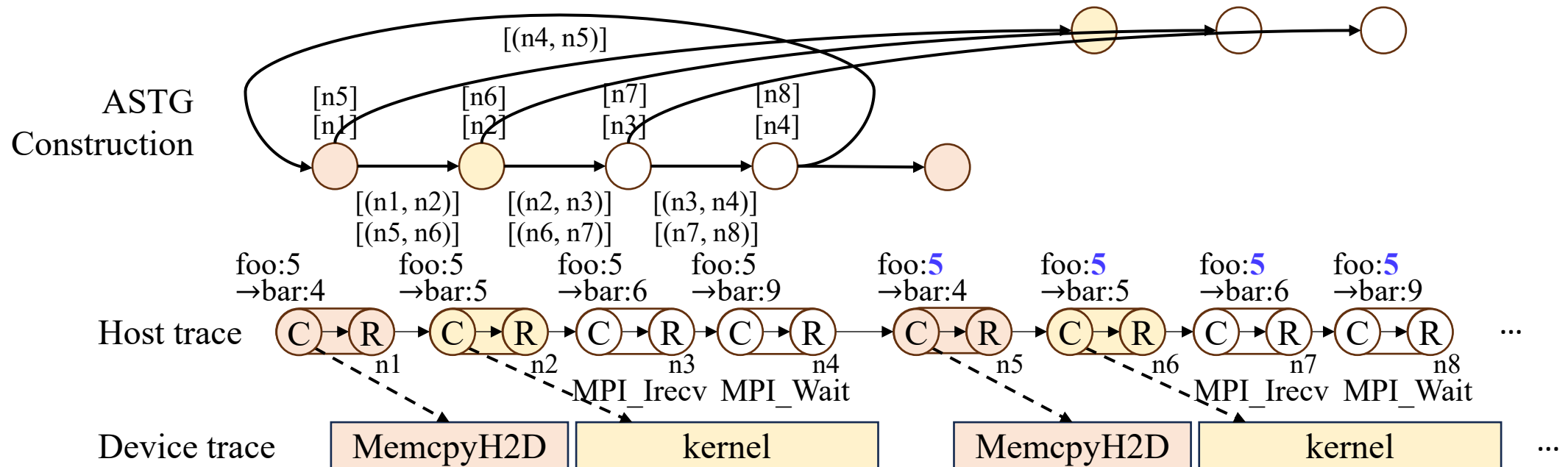
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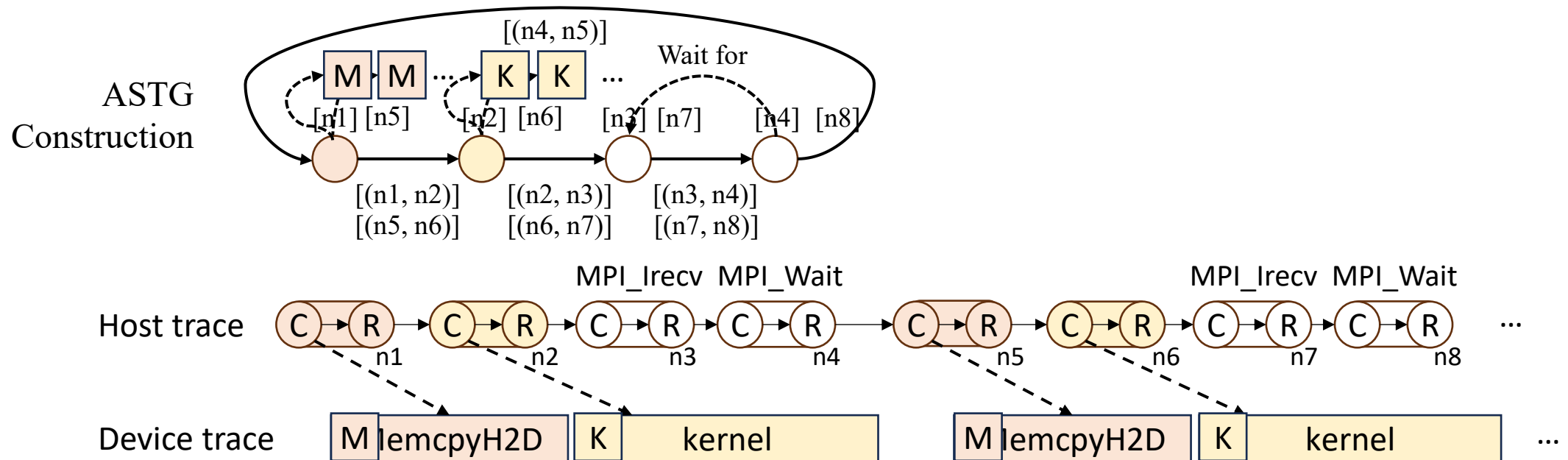
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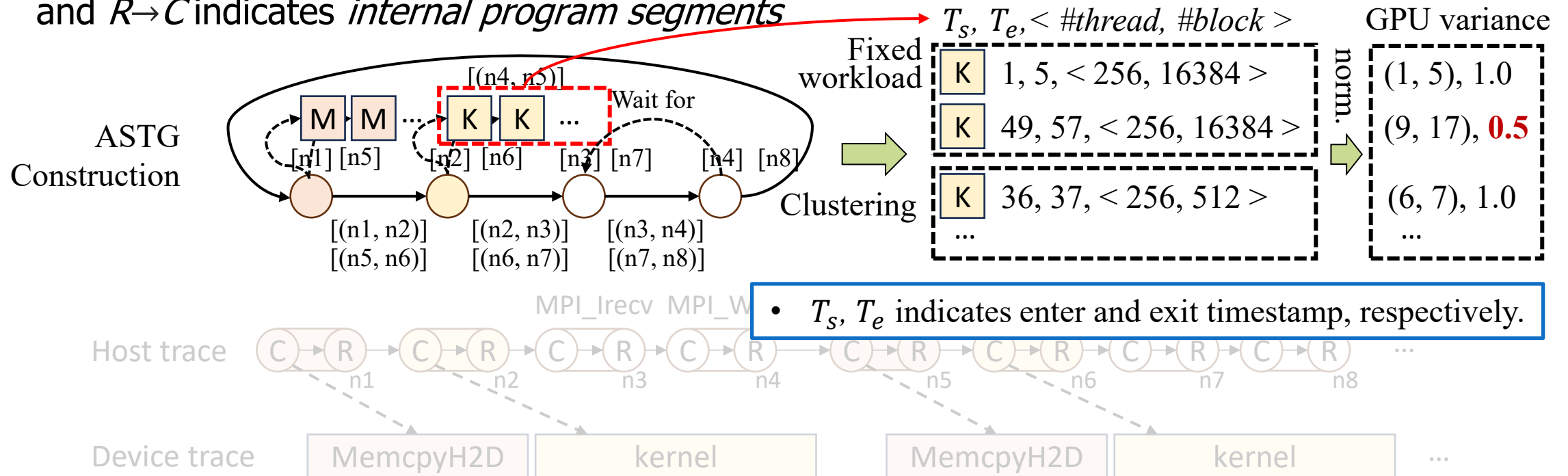
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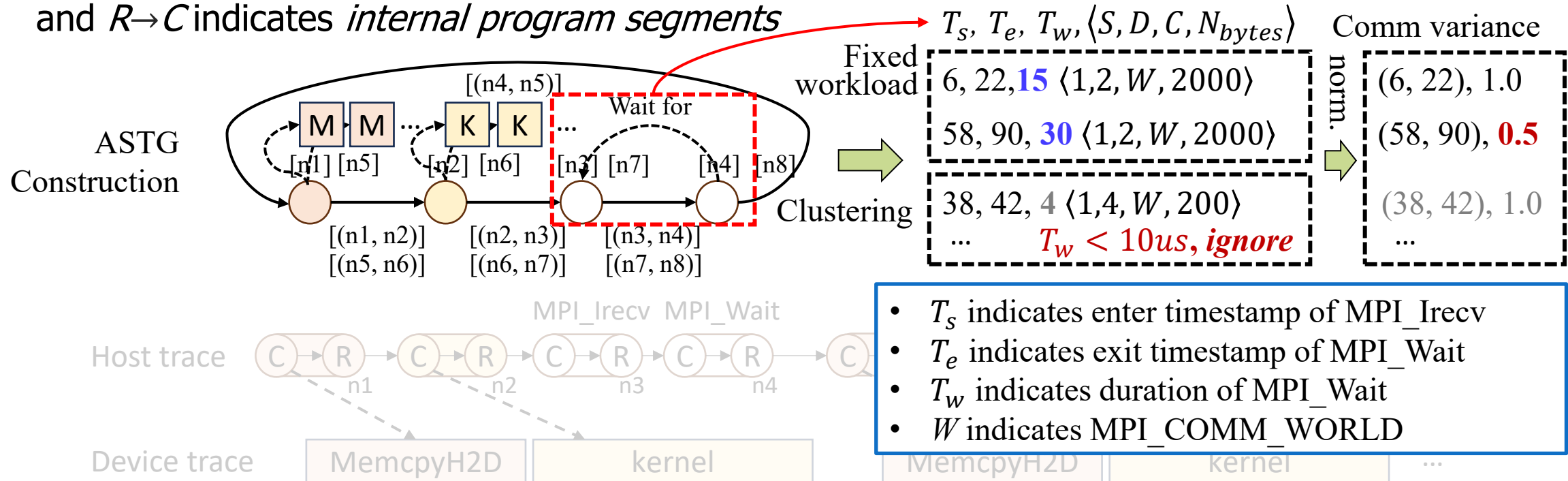
ASTG-based Performance Variance Detection

- Based on the constructed ASTG, GVARP can identify the **fixed workload** program segments for further performance variance detection
 - CPU-GPU data transfer (*orange icons*), GPU kernel launch (*yellow icons*) and MPI communication (*white icons*)
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ASTG-based Performance Variance Detection

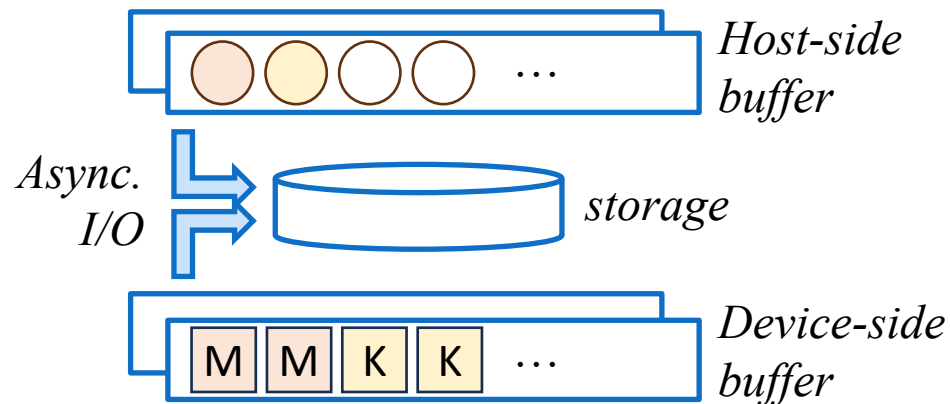
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Implementation - Low cost at scale

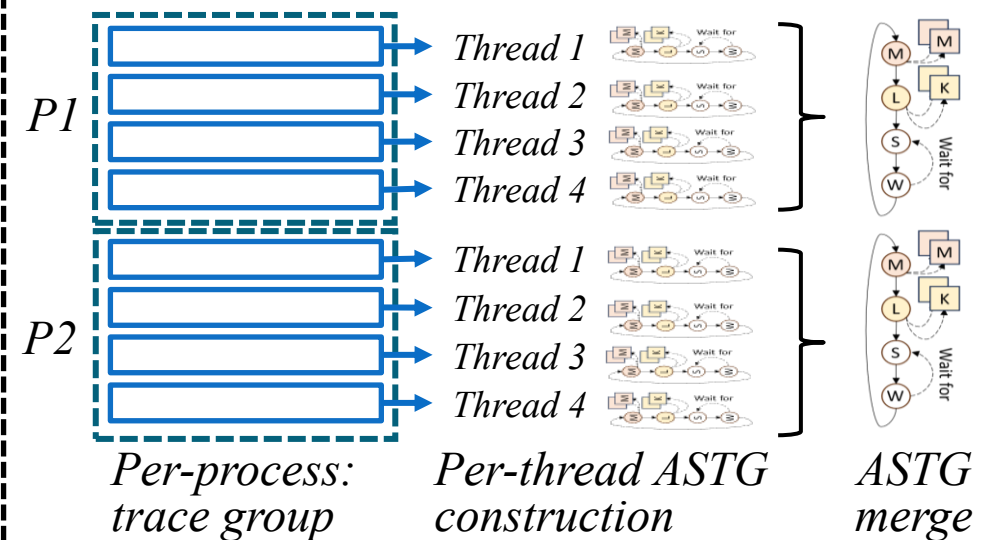
- For detecting performance variances at scale, GVARP implements the above methods efficiently with the following techniques:

1) Tracing efficiency:



Implement **host-device dual buffer enabled asynchronous event tracing** within GVARP library interception

2) Analysis efficiency:



Implement **communication-free MPI and OpenMP hybrid parallelization** for efficient ASTG construction

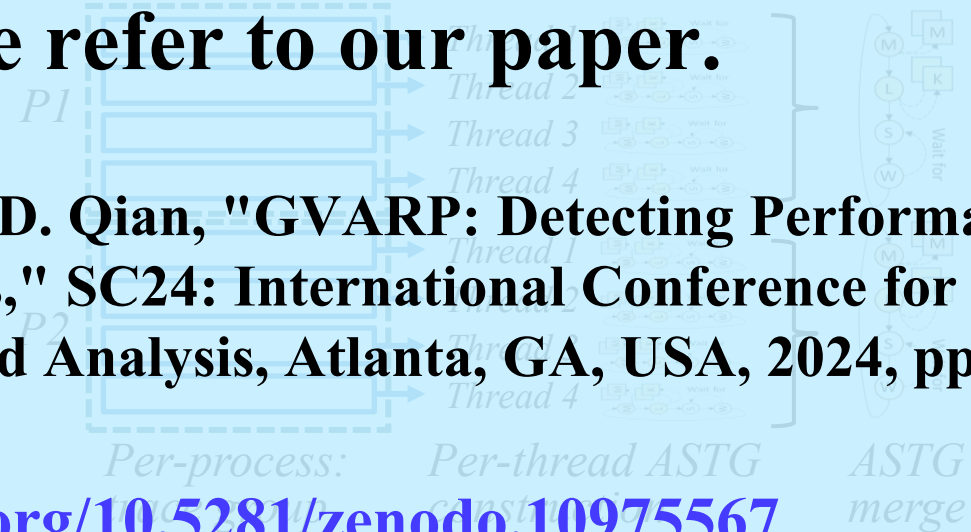
Implementation - Low cost at scale

- For detecting performance variances at scale, GVARP implements the above methods efficiently with the following techniques:

For more details, please refer to our paper.

X. You, Z. Xuan, H. Yang, Z. Luan, Y. Liu and D. Qian, "GVARP: Detecting Performance Variance on Large-Scale Heterogeneous Systems," SC24: International Conference for High Performance Computing, Networking, Storage and Analysis, Atlanta, GA, USA, 2024, pp. 1-13.

GVARP is available: <https://doi.org/10.5281/zenodo.10975567>



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Evaluation Setup

- We evaluate GVARP on an AMD GPU cluster with up to 16,000 GPUs
- 3 representative GPU-accelerated HPC program
 - (1) HPCG: a high-performance conjugate gradients benchmark
 - (2) ANT-MOC: a scalable neutron transport equation solver
 - (3) LAMMPS: a widely adopted molecular dynamics simulator in various domains
- Both ANT-MOC and LAMMPS achieves large scale parallelization of **16,000 MPI processes and 16,000 GPUs**

Platform	GPU Cluster
CPU	AMD Zen-based processor @ 2.5GHz
GPU	4 AMD Instinct M160 GPUs
Cores	32
Memory	128 GB (host), 16 GB (GPU)
Network	200 Gbps HDR InfiniBand network
Storage	> 200 Gbps
Software	GCC 9.3.1, ROCM \geq 3.9, OpenMPI 4.0.4

Detection Coverage

- We evaluate with 128 processes + 128 GPUs (small scale varification) and 16,000 processes+16,000 GPUs (whole machine scale)

Program	Scale	Sync-only	Detailed Coverage				Coverage	
		Comm.	Host Comp.	Comm.	Device Comp.	Host-device Data Transfer	Host	Device
HPCG	128	0.00%	70.60%	0.02%	0.01%	0.00%	70.62%	0.01%
ANT-MOC	128	0.00%	3.05%	2.08%	67.52%	6.20%	5.13%	73.72%
LAMMPS	16,000	0.21%	9.45%	0.32%	0.18%	4.46%	9.77%	4.64%
ANT-MOC	16,000	0.00%	9.69%	0.01%	0.92%	0.82%	9.70%	1.74%

GVARP can identify some **asynchronous communications** as fixed-workload segments through its ASTG-based communication workload identification

GVARP can identify both GPU **data transfer and computation** as probes for variance detection

Overhead

- We execute at least 3 times for each evaluated program and choose the fastest execution time as the reported evaluation results

Program	Scale	Overhead		
		Time	Storage	Analysis (s)
HPCG	128	1.00×	8.9 GB	877.5
ANT-MOC	128	1.00×	2.0 GB	447.04
LAMMPS	16,000	1.14×	70.0 GB	288.04
ANT-MOC	16,000	1.16×	60.0 GB	390.51

*Analysis
with 1 node*

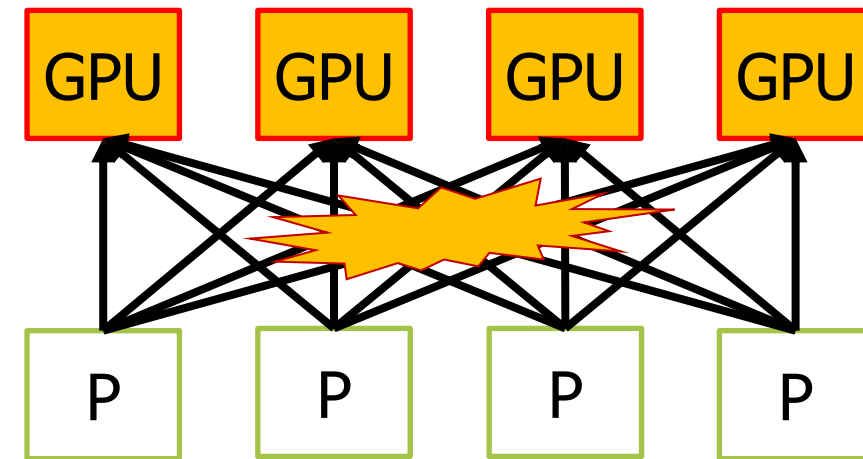
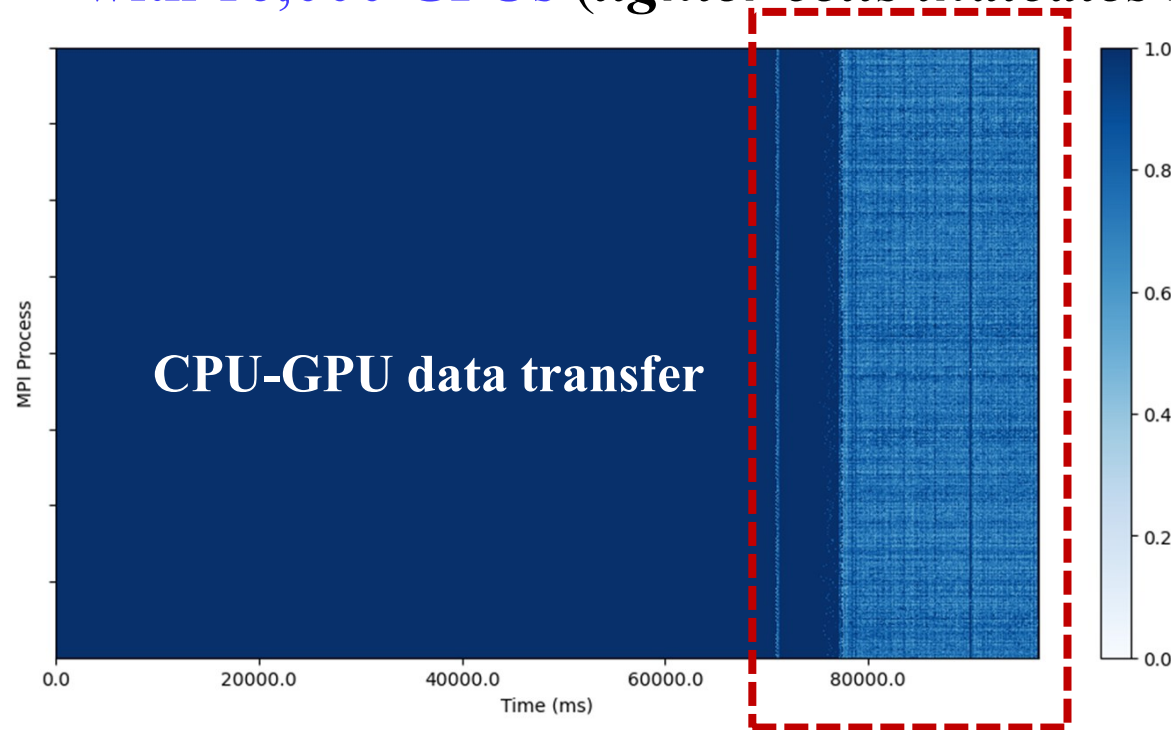
*Analysis
with 4 node*

Such **low time overheads** can be attributed to the asynchronous event tracing techniques adopted in GVARP implementation.

GVARP requires several minutes for **performance variance detection analysis**, which is also **acceptable** to perform in free debug nodes

Case Study: Detection of Launching Problem (LAMMPS)

- The performance variance detected in **host-device data transfer** for executing **LAMMPS with 16,000 GPUs** (*lighter cells indicates more severe performance variances*)

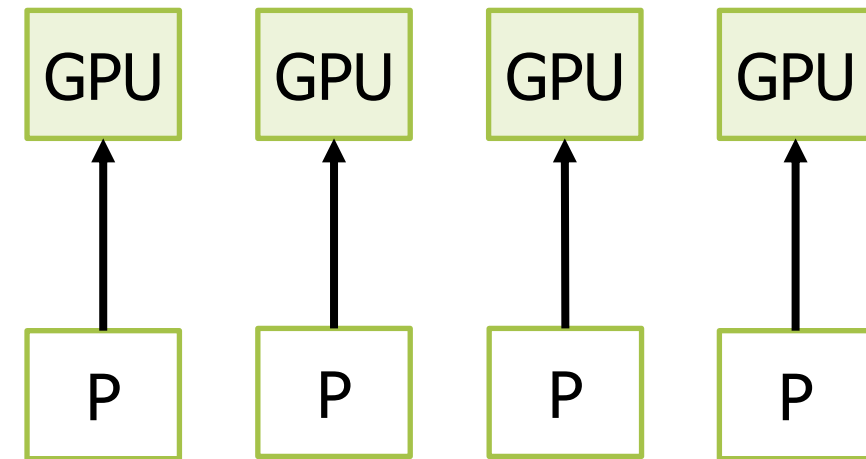
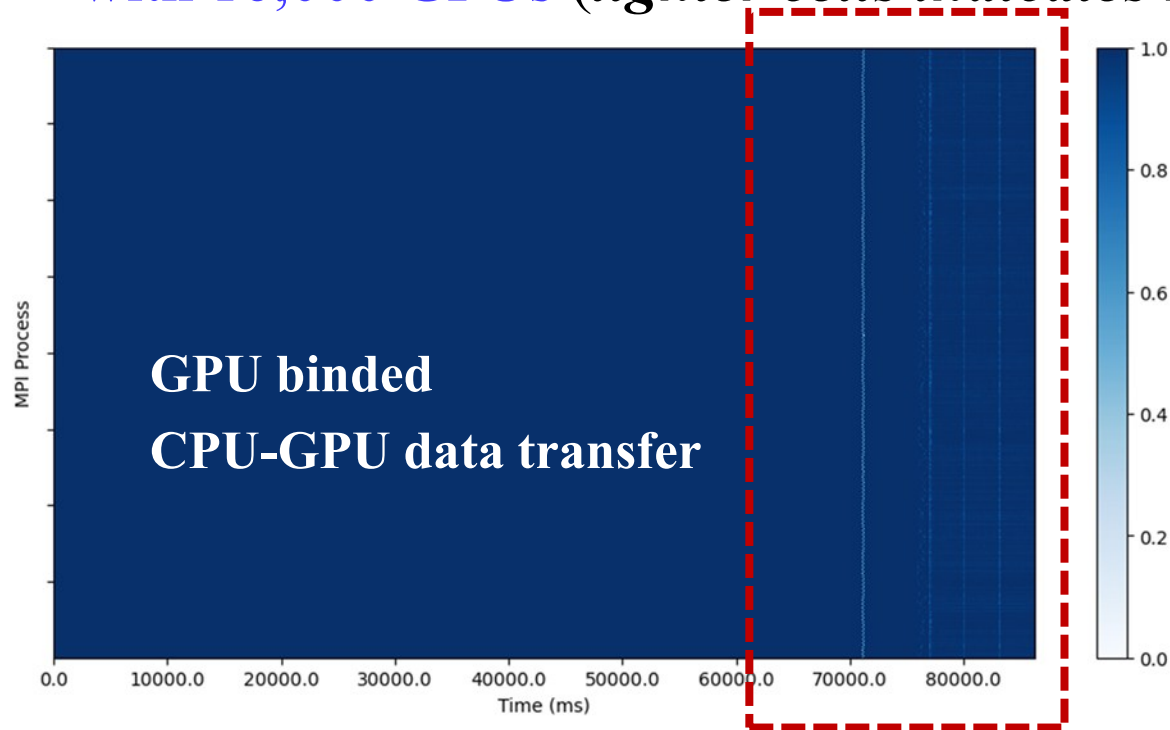


LAMMPS wrongly binds the same GPU for acceleration with improper launching configurations

- Such performance variance must come from strong interference along PCIe data transition

Case Study: Detection of Launching Problem (LAMMPS)

- The performance variance detected in **host-device data transfer** for executing **LAMMPS with 16,000 GPUs** (*lighter cells indicates more severe performance variances*)



Properly bind from launch configuration

- Such performance variance must come from strong interference along PCIe data transition
- **After properly binded, we achieve 1.56x performance speedup**

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 - Installation
 - Case Study – ANT-MOC
 - Case Study – LAMMPS

Installation - GVARP

■ Install with source code:

- Dependencies: git, gcc >=12, cmake >=3.20, libunwind, ... (*can install with spack*)
- Source Code: `git clone https://github.com/buaa-hipo/MSToolkit.git`
- Compilation Instruction: `cd MSToolkit && ./build.sh`
- Configure the Path: `source env.sh`

■ Use pre-installed version in tutorial cluster:

- Configure the Tool Path: `source ~/GVARP-Tutorial/examples/ANT-MOC/setup-env.sh`
`# source ~/GVARP-Tutorial/examples/LAMMPS/setup-env.sh`
`conda activate mstoolkit # load python env to dump figures`

■ Instruction to analyze the target program:

- Tracing with *jsirun*: `mpirun -n ${NP} jsirun <tool options> -- <EXE> <ARGS>`
- Variance detection: `variance_analysis -i <TRACE DIR> -o <RESULT_DIR>`

GVARP – More usage details

- **Support various configurations for *jsirun* to collect data including:**

- MPI events with parameters (*enabled by default*)
- ROCM/HIP API calls & device events (*--accl*)
- Backtrace collection (*--backtrace*)
- Performance counters (*--pmu*), events are defined in environment variable:

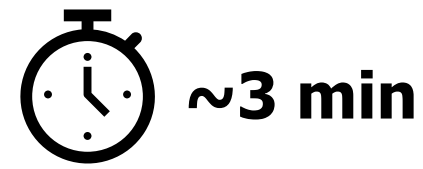
```
export JSI_COLLECT_PMU_EVENT=PAPI_TOT_INS,PAPI_L1_DCA
```

- ...

- **Performance variance detection with *variance_analysis*:**

- Resolution (ms) for heatmap generation (*-r, --resolution arg*), default is **100ms**
- One can also change the reference PMU events for host computation workload estimation (*-m, --reference-metric arg*), default is **PAPI_TOT_INS**

Case Study: ANT-MOC: Tracing



- Get the tutorial cases for ANT-MOC

```
cp -r /public/home/dfcs2025/GVARP-Tutorial/examples/ANT-MOC ./
```

- Tracing for ANT-MOC normal execution

Modify the
Job Name

```
cd ANT-MOC/run-ori  
./slurm-tool.job # generate & submit ANT-MOC jobs with and without tool
```

```
#!/bin/bash  
NTASKS=16  
JOBNAME="MOC-blk"  
RUN_DIR=`dirname $0`  
echo "TASK MOC C5G7 TEST START NTASK=$NTASKS "  
NEWMOC=/public/home/buaa_hipo/CLUSTER25-  
Tutorial/app/ANT-MOC/ANT-MOC/build/run/newmoc  
MEASUREMENT_DIR_ORI=measurement/measurement-antmoc-ori  
nowdate=$(date +%Y_%m_%d %H %M %S)  
echo $nowdate  
sbatch << END  
#!/bin/bash  
#SBATCH -J $JOBNAME  
#SBATCH -o log/c5g7/c5g7-$NTASKS-%j-$nowdate.log  
#SBATCH -e log/c5g7/c5g7-$NTASKS-%j-$nowdate.err  
#SBATCH -p test  
#SBATCH --cpus-per-task=7
```

Modify the TRACE
FILE PATH

```
#SBATCH --ntasks-per-node=4  
#SBATCH --gres=dcu:4  
#SBATCH --mem=100GB  
#SBATCH -n $NTASKS  
cd $RUN_DIR && source $RUN_DIR/../setup-env.sh  
export OMP_NUM_THREADS=1  
export JSI_BACKTRACE_MAX_DEPTH=5  
export JSI_COLLECT_PMU_EVENT=PAPI_TOT_INS,PAPI_L1_DCA  
rm -rf $MEASUREMENT_DIR_ORI  
/usr/bin/time -v mpirun -n $NTASKS $NEWMOC --  
config="./config.vaml"  
/usr/bin/time -v mpirun -n $NTASKS jsirun --accl --  
backtrace --pmu -o $MEASUREMENT_DIR_ORI -- $NEWMOC --  
config="./config.yaml"
```

END

Unoptimize
d time

Profiling time

Slides is available at tutorial home page:

<https://buaa-hipo.github.io/blog/mstoolkit-tutorial-cluster25/>



Case Study: ANT-MOC: Analysis of normal execution ~2 min

- Load the mstoolkit environments for variance analysis

```
conda activate mstoolkit  
source ../setup-env.sh
```

- Submit an analysis job and the result file is located in folder ***variance/***

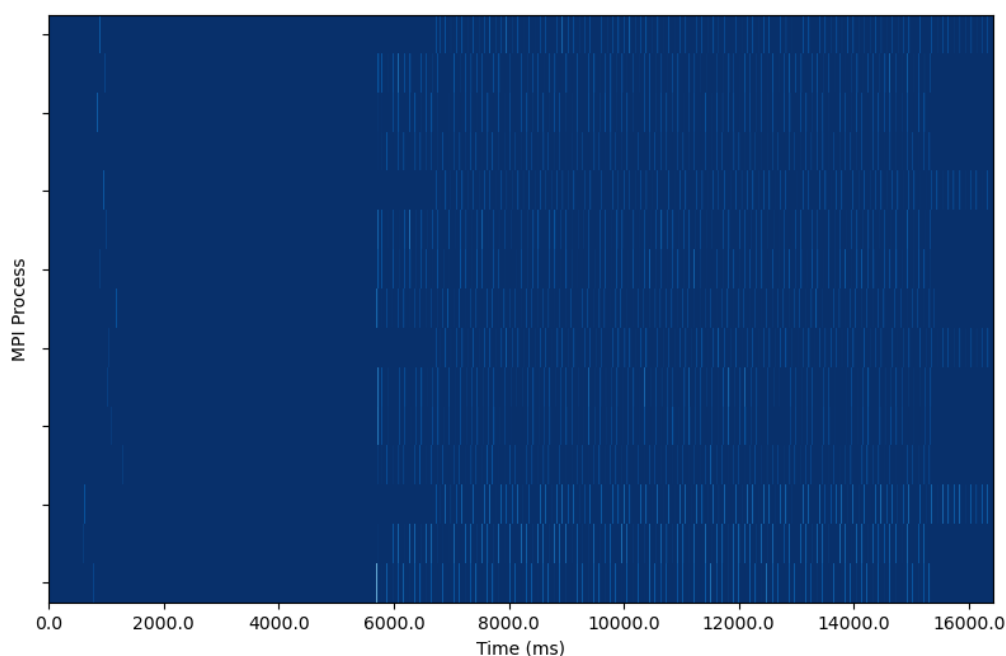
```
srun -n 1 --cpus-per-task 2 -p sep2 --exclusive --mem=100GB variance_analysis -i  
measurement/measurement-antmoc-ori -o variance -f --reference-metric-add PAPI_L1_DCA  
--resolution 10
```

- ***Contains 5 result files in csv format:*** *accl_calc_heat.csv, accl_memcpy_heat.csv, calc_heat.csv, comm_heat.csv, host.csv*
- Indicates analysis results for *device computation, host-device transfer, host computation, communication* and *process-host mapping* information, respectively
- Draw heatmap figures with the provided script

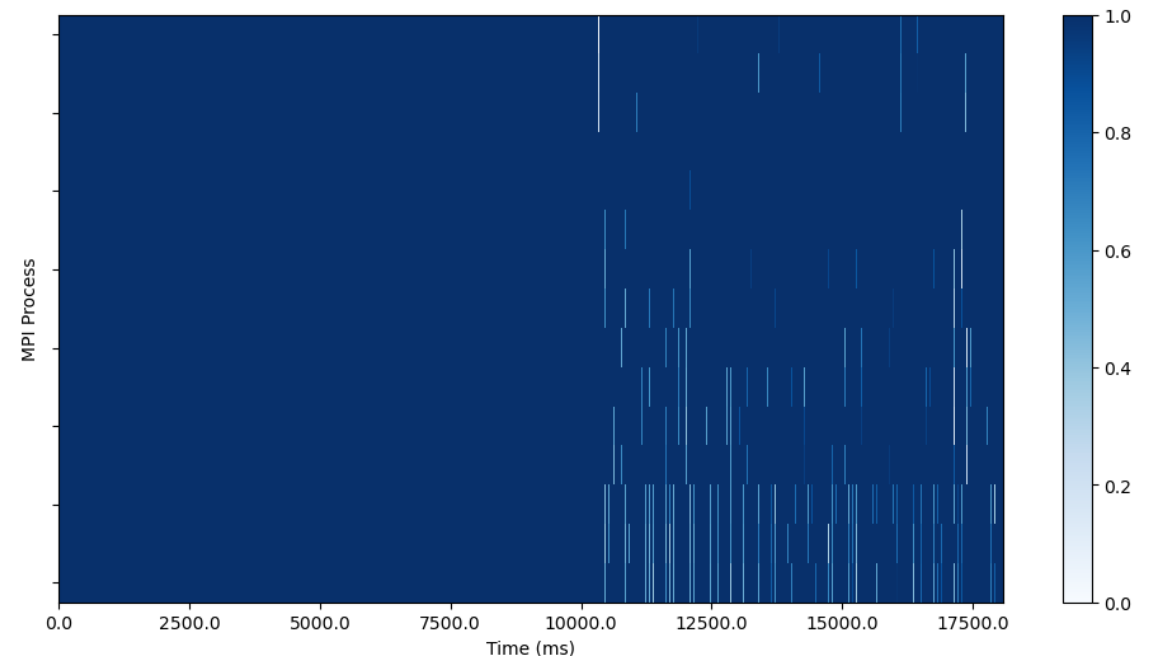
```
HEATMAP_PY=$MSTOOLKIT_PATH/scripts/analysis/variance/heatmap.py  
python $HEATMAP_PY --input variance --output figure
```

Case Study: ANT-MOC: Analysis of normal execution

- Resulting files are located in the folder ***figure/***
 - ***Contains 4 result figures:*** *accl_calc.png*, *accl_memcpy.png*, *calc.png*, *comm.png*
 - Indicates analysis results for *device computation*, *host-device transfer*, *host computation*, and *communication*, respectively
 - ***The lighter indicates worser performance***



accl_calc.png



comm.png

Case Study: Inject Device Computation Workloads



- Now try to inject device-only computation workload along with ANT-MOC execution to simulate severe device-side performance variance.
- Injected computation-intensive kernel
 - Located in **run-accl-calc/inject-accl-calc/stress.cpp**
 - **Injected after 20 seconds, last for 20 seconds**
- Provide a reference job submission scripts for *inject & tracing*

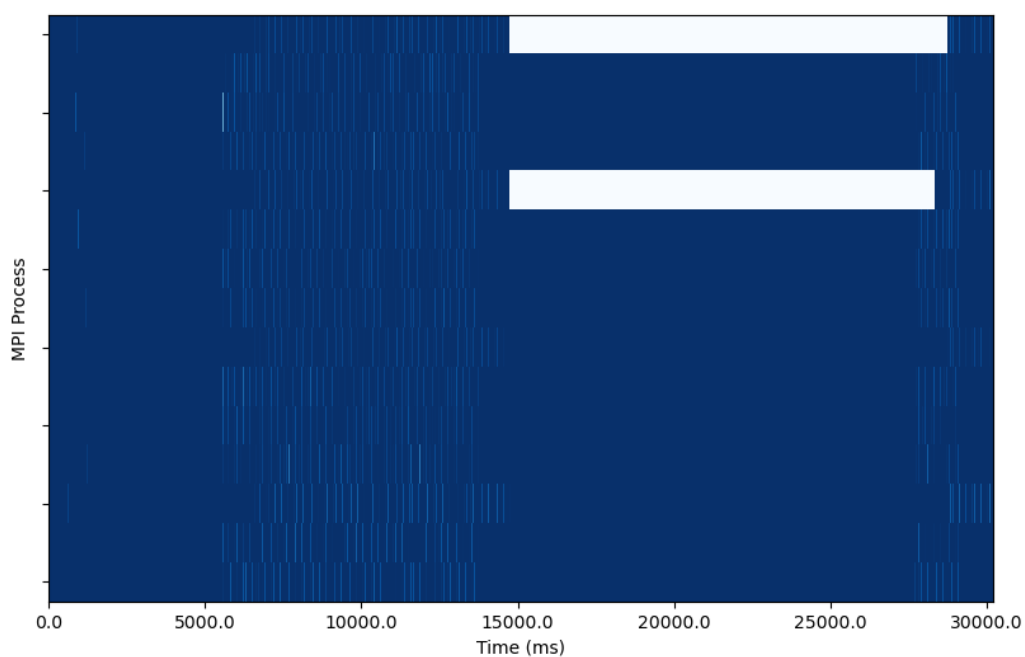
```
cd <path/to/ANT-MOC>  
cd run-accl-calc  
./slurm-tool.job # inject device-only computation & trace for further analysis
```

- Once the tracing the finished, run the analysis script for heatmap figures

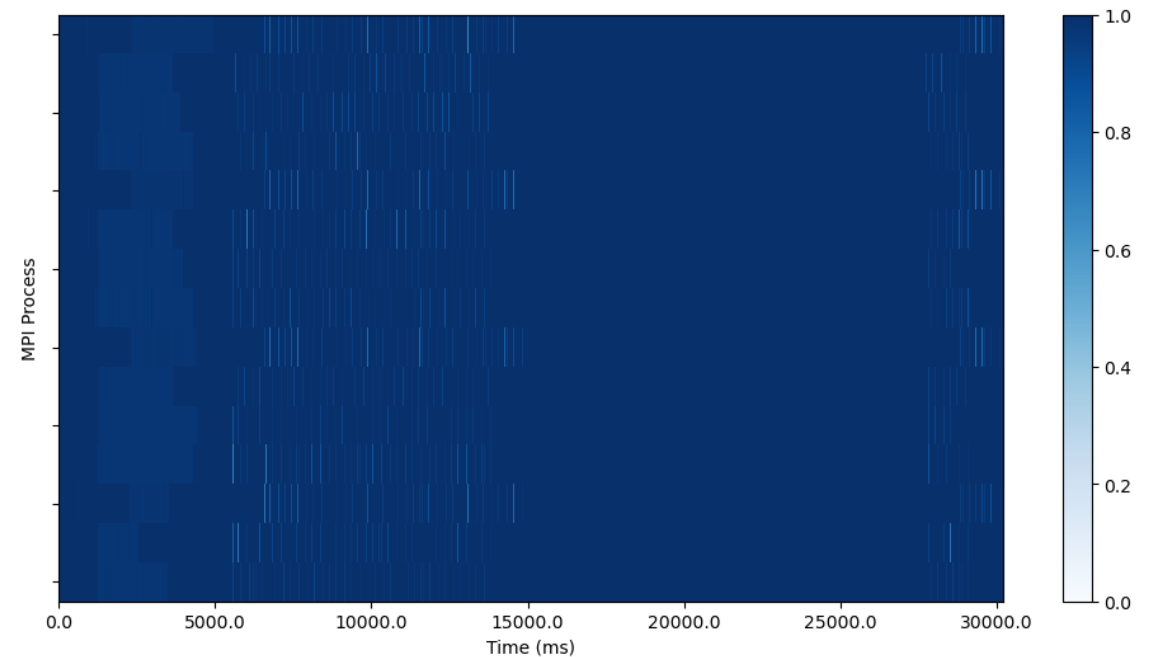
```
conda activate mstoolkit # make sure the python environment is ready  
./run_analysis.sh # the previous analysis commands are wrapped into the given scripts
```

Case Study: Inject Device Computation Workloads

- Resulting files are located in the folder ***figure/***
 - ***Target variance only appears in accl_calc.png***
 - ***The lighter indicates worser performance***



accl_calc.png



accl_memcpy.png

Case Study: Inject Host-Device Data Transfer



- Now try to inject host-device data transfer workload along with ANT-MOC execution to simulate severe PCIe performance variance.
- Injected computation-intensive kernel
 - Located in **run-accl-mem/inject-accl-mem/inject_accl_mem.cpp**
 - **Injected after 0 seconds, last for 60 seconds**
- Provide a reference job submission scripts for *inject & tracing*

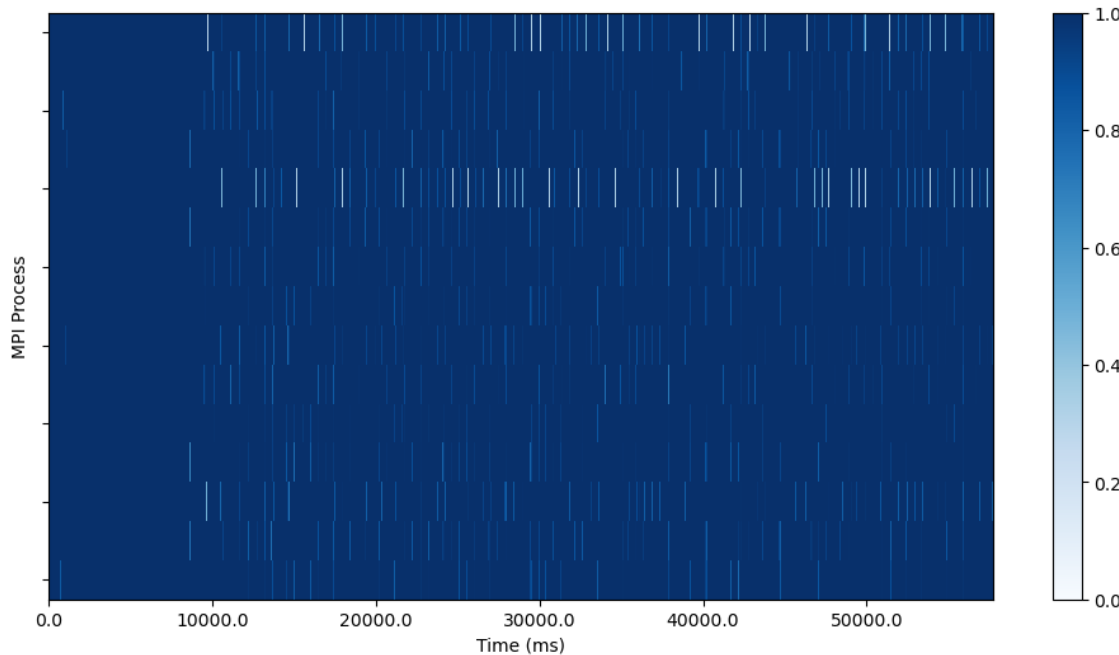
```
cd <path/to/ANT-MOC>
cd run-accl-mem
./slurm-tool.job # inject host-device data transfer & trace for further analysis
```

- Once the tracing the finished, run the analysis script for heatmap figures

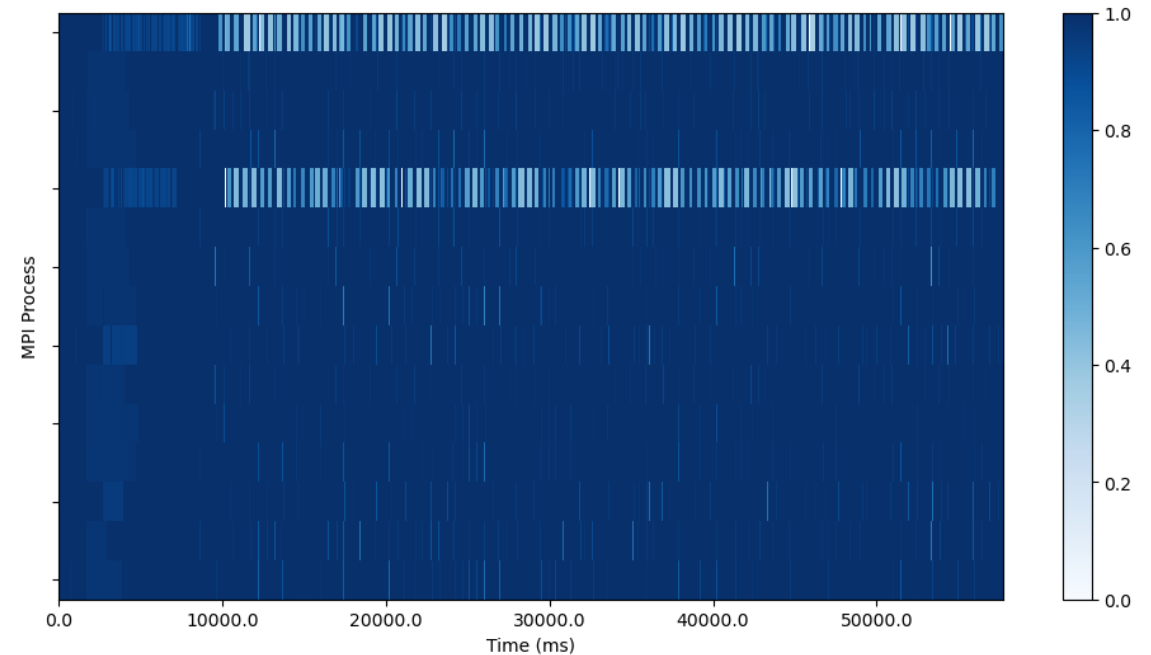
```
conda activate mstoolkit # make sure the python environment is ready
./run_analysis.sh # the previous analysis commands are wrapped into the given scripts
```

Case Study: Inject Host-Device Data Transfer

- Resulting files are located in the folder ***figure/***
 - ***Target variance only appears in accl_memcpy.png***
 - ***The lighter indicates worser performance***



accl_calc.png



accl_memcpy.png

Case Study: Inject Host Computation



- Now try to inject host computation workload along with ANT-MOC execution to simulate severe host-side performance variance.
- Injected computation-intensive kernel
 - Located in **run-calc/inject-calc/inject.cpp**
 - **Injected after 0 seconds, last for 60 seconds**
- Provide a reference job submission scripts for *inject & tracing*

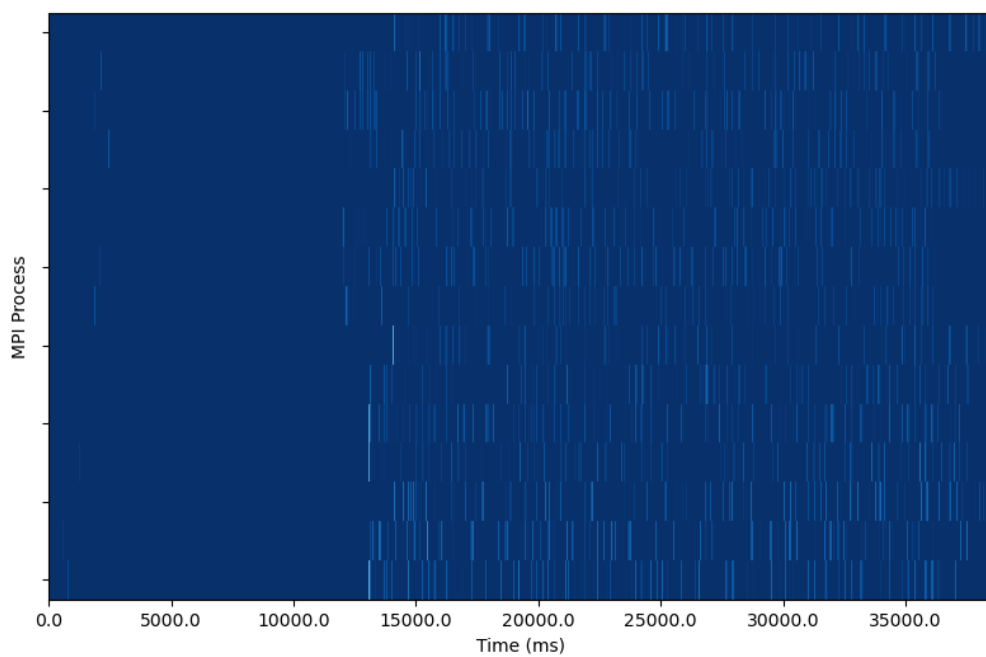
```
cd <path/to/ANT-MOC>  
cd run-calc  
./slurm-tool.job # inject host computation & trace for further analysis
```

- Once the tracing the finished, run the analysis script for heatmap figures

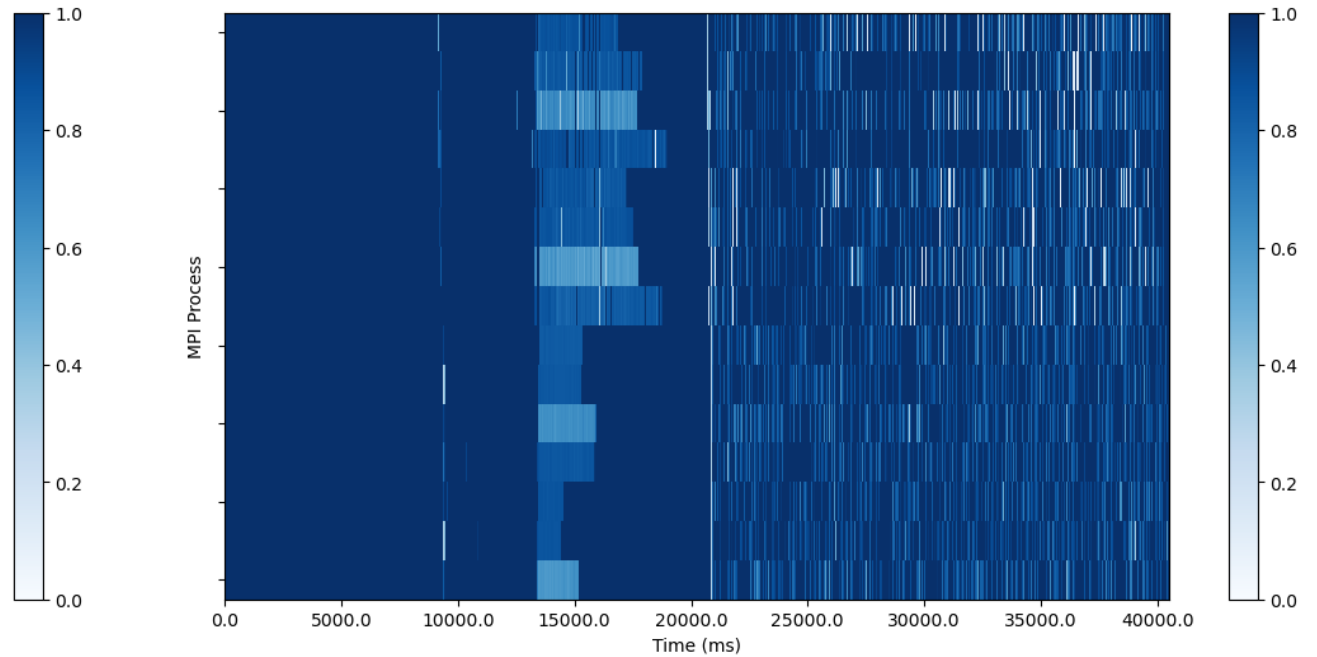
```
conda activate mstoolkit # make sure the python environment is ready  
./run_analysis.sh # the previous analysis commands are wrapped into the given scripts
```


Case Study: Inject Host Computation

- Resulting files are located in the folder ***figure/***
 - ***Target variance only appears in calc.png***
 - ***The lighter indicates worser performance***



accl_calc.png



calc.png

Case Study: LAMMPS real case



- Get the tutorial cases for LAMMPS

```
cp -r /public/home/dfcs2025/GVARP-Tutorial/examples/LAMMPS ./ && cd LAMMPS/run-1
```

- Submit LAMMPS jobs without tool (***default execution***)

```
sbatch slurm-nobind-ori.job
```

- Submit LAMMPS jobs with tool (***tracing for data collection***)

```
sbatch slurm-nobind-tool.job
```

```
#!/bin/bash
#SBATCH -J LMP-NOBIND-TOOL
#SBATCH -o log/lmp-nobind-tool-%j.log
#SBATCH -e log/lmp-nobind-tool-%j.err
#SBATCH -p test
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=4
#SBATCH --gres=dcu:4
#SBATCH -n 16
export OMP_NUM_THREADS=1
export JSI_BACKTRACE_MAX_DEPTH=5
export JSI_COLLECT_PMU_EVENT=PAPI_TOT_INS,PAPI_L1_DCA
```

```
source /public/home/dfcs2025/GVARP-
Tutorial/.test/LAMMPS/setup-env.sh
```

```
rm -rf measurement/measurement-nobind
```

```
/usr/bin/time -v mpirun -n 16 jsirun --accl --backtrace
--pmu -o measurement/measurement-nobind -- lmp_mpi -sf
gpu -pk gpu 1 -i in.balance.static.4N16DCU
```

Use DTK23
version

Tracing
with ***jsirun***

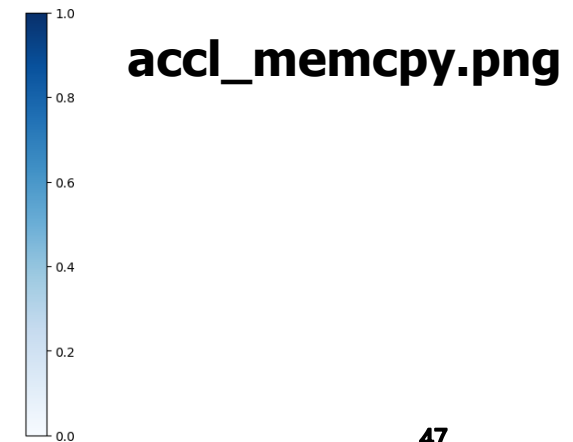
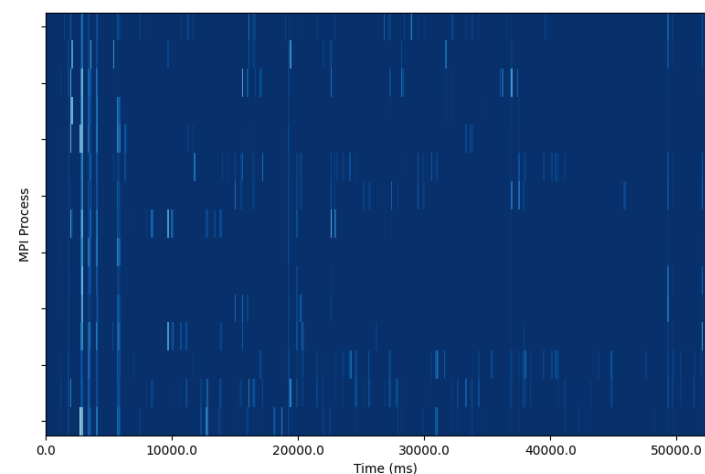
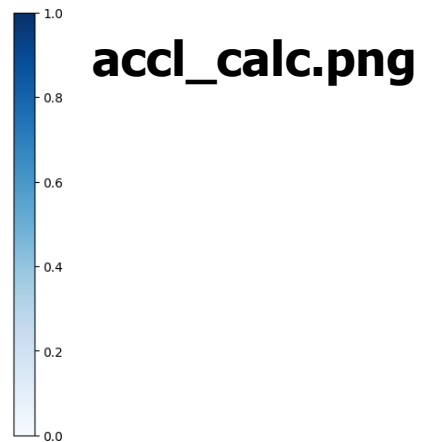
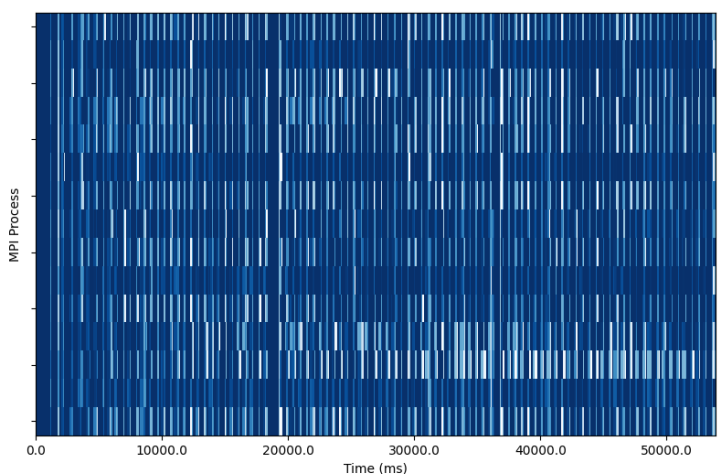
Case Study: LAMMPS real case

- Load the mstoolkit environments for variance analysis

```
conda activate mstoolkit  
source ../setup-env.sh
```

- Submit an analysis job and the result file is located in folder ***figure-nobind/***

```
srun -n 1 --cpus-per-task 2 -p sep2 --exclusive --mem=100GB variance_analysis -i  
measurement/measurement-nobind -o variance-nobind -f  
HEATMAP_PY=$MSTOOLKIT_PATH/scripts/analysis/variance/heatmap.py  
python $HEATMAP_PY --input variance-nobind --output figure-nobind
```



Case Study: LAMMPS real case

- Check for log: *log/imp-nobind-tool-<slurm job id>.log*

```
LAMMPS (2 Aug 2023)
  using 1 OpenMP thread(s) per MPI task
```

```
...
```

```
-----
- Using acceleration for lj/cut:
-   with 4 proc(s) per device.
-   with 1 thread(s) per proc.
- Horizontal vector operations: ENABLED
- Shared memory system: No
-----
```

```
Device 0: Device 66a1, 64 CUs, 16/16 GB, 1.7 GHZ (Mixed Precision)
-----
```

```
Initializing Device and compiling on process 0...Done.
Initializing Device 0 on core 0...Done.
Initializing Device 0 on core 1...Done.
Initializing Device 0 on core 2...Done.
Initializing Device 0 on core 3...Done.
```

```
...
```

Bind to the same GPU!

Case Study: LAMMPS real case

■ Bind GPU with its MPI rank via numactl && HIP_VISIBLE_DEVICES

```
#!/bin/bash
APPCMD="$*"
lrank=$(expr $OMPI_COMM_WORLD_LOCAL_RANK % 4)
case ${lrank} in
[0])
export HIP_VISIBLE_DEVICES=0
export UCX_NET_DEVICES=mlx5_0:1
export UCX_IB_PCI_BW=mlx5_0:50Gbs
numactl --cpunodebind=0 --membind=0 ${APPCMD}
;;
[1])
export HIP_VISIBLE_DEVICES=1
export UCX_NET_DEVICES=mlx5_1:1
export UCX_IB_PCI_BW=mlx5_1:50Gbs
numactl --cpunodebind=1 --membind=1 ${APPCMD}
;;
[2])
export HIP_VISIBLE_DEVICES=2
export UCX_NET_DEVICES=mlx5_2:1
export UCX_IB_PCI_BW=mlx5_2:50Gbs
numactl --cpunodebind=2 --membind=2 ${APPCMD}
;;
[3])
export HIP_VISIBLE_DEVICES=3
export UCX_NET_DEVICES=mlx5_3:1
export UCX_IB_PCI_BW=mlx5_3:50Gbs
numactl --cpunodebind=3 --membind=3 ${APPCMD}
;;
esac
```

bind.sh

```
#!/bin/bash
#SBATCH -J LMP-BIND-TOOL
#SBATCH -o log/lmp-bind-ori-%j.log
#SBATCH -e log/lmp-bind-ori-%j.err
#SBATCH -p test
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=4
#SBATCH --gres=dcu:4
#SBATCH -n 16
#
export OMP_NUM_THREADS=1
export JSI_BACKTRACE_MAX_DEPTH=5
export
JSI_COLLECT_PMU_EVENT=PAPI_TOT_INS,PAPI_L1_DCA

#cd /public/home/buaa_hipo/CLUSTER25-
Tutorial/app/LAMMPS/run-1

module load apps/lammps-DCU/2Aug2023/hpcx-2.7.4-
dtk23.10

/usr/bin/time -v mpirun -n 16 ./bind.sh lmp_mpi -
sf gpu -pk gpu 1 -i in.balance.static.4N16DCU
```

Bind to the different GPU

slurm-bind-ori.job

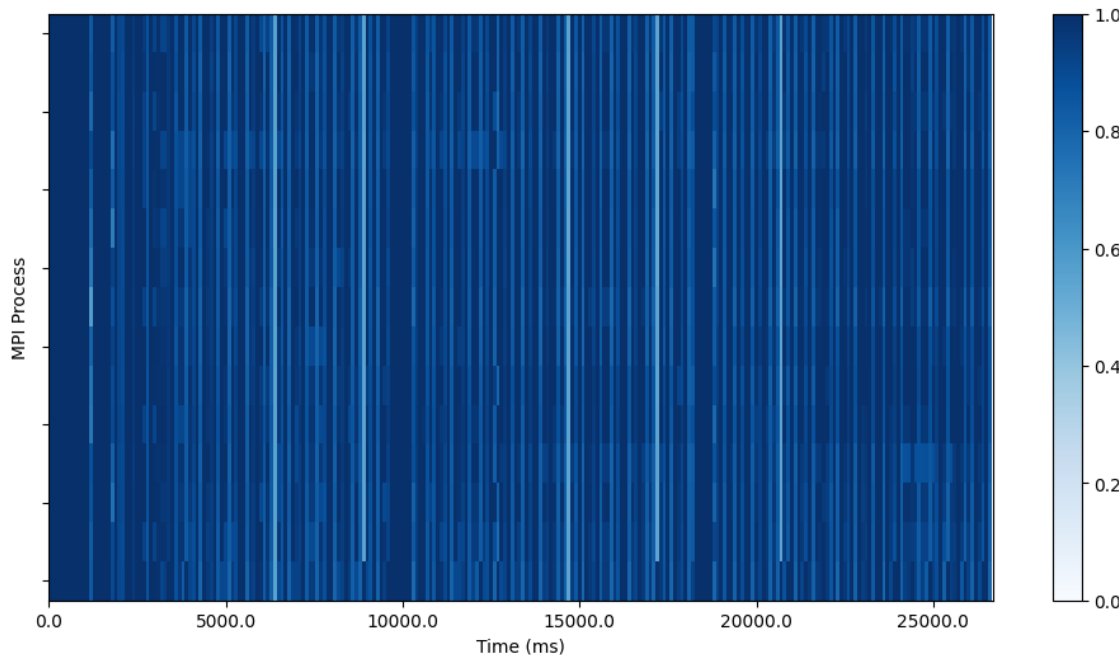
Case Study: LAMMPS real case

- Submit the optimized configuration && tracing for validation

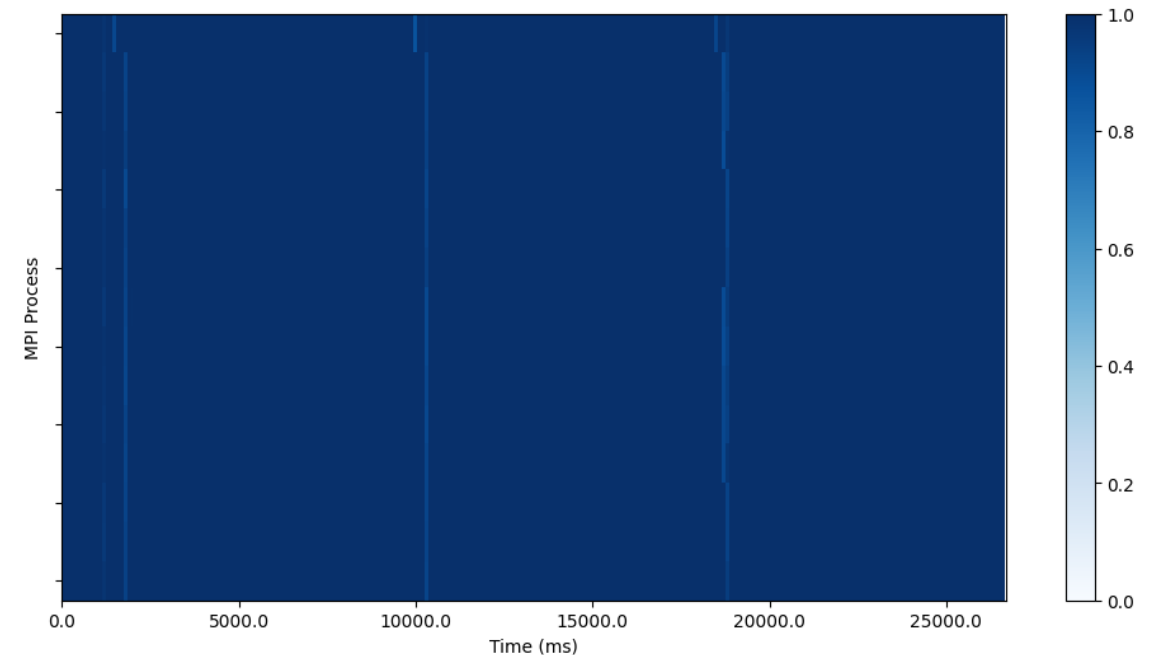
```
sbatch slurm-bind-ori.job  
sbatch slurm-bind-tool.job
```

- Run analysis when the job is finished and the tracing data is ready

```
srun -n 1 -p test --mem=100GB variance_analysis -i measurement/measurement-bind -o variance-bind -f  
python $ HEATMAP_PY --input variance-bind --output figure-bind
```



accl_calc.png



accl_memcpy.png

Thanks! Q&A

Contact: youxin2015@buaa.edu.cn