

# Building a Future of HPC Performance Engineering Rooted in Data, Tools, and Trust

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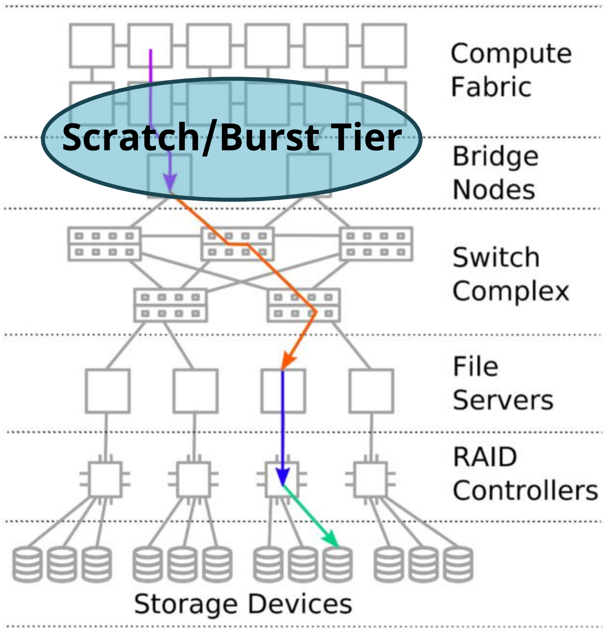
# Motivation
## *Heterogeneous and Complex HPC Infrastructures*

- HPC infrastructure *too complex*, humans are *overwhelmed*
- Complexity and scope increase the *urgency*
  - *New computational paradigms* (AI/ML apps vs. BSP-style HPC)
  - *New architectural directions* (e.g., IPU, RISC-V, data flow)
  - *Heterogeneity overall*: node architectures, within the system, storage and parallel file system during application design (e.g., ML within HPC applications)
  - *New operations paradigms* (e.g., cloud, container)
  - Simplistic approaches to increasing compute demand result in *unacceptable power costs*
- Difficult for humans to optimally adapt applications to systems and to detect and diagnose vulnerabilities





Carns, P., 2023. *HPC Storage: Adapting to Change*. Keynote at REX-IO'23 Workshop.

Ciorba, F., 2023. *Revolutionizing HPC Operations and Research*. Keynote at HPCMASPA'23 Workshop.

B. Settlemyer, G. Amvrosiadis, P. Carns and R. Ross, 2021. *It's Time to Talk About HPC Storage: Perspectives on the Past and Future*, in Computing in Science & Engineering, vol. 23, no. 6, pp. 63-68.

# Vision: From Data to Decisions

*Holistic Monitoring for Intelligent HPC Operations*

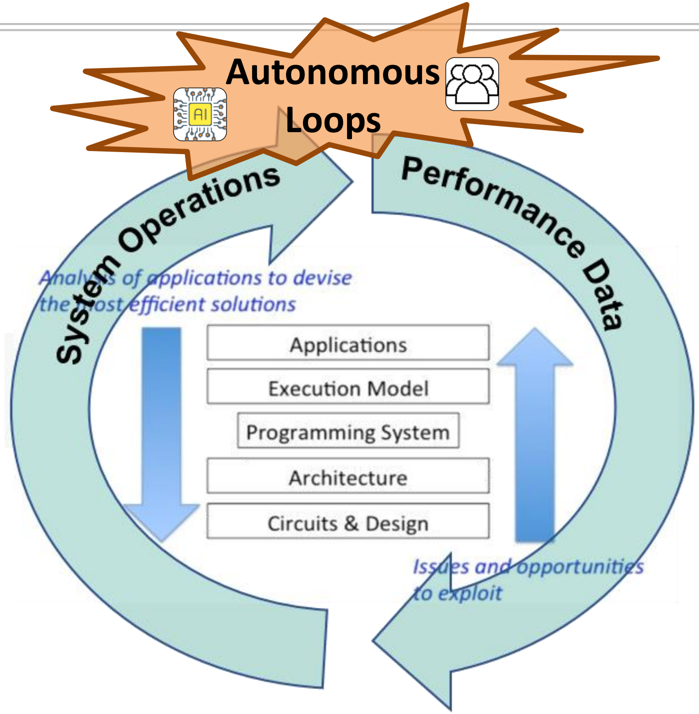
**What We Need:**

- Continuous monitoring, archiving, and analysis of operational + performance data
- Unified visibility into applications, system software, and hardware layers

**Why It Matters:**

- Enables automated feedback loops using AI/ML
- Supports dynamic workload & architecture analysis
- Powers adaptive, actionable responses

**Goal:** Efficient, explainable HPC operations driven by *autonomous analyze-feedback-response loops*





Gentile, A., 2021. *Enabling Application and System Data Fusion*. Keynote at MODA'21 Workshop.

Ciorba, F., 2023. *Revolutionizing HPC Operations and Research*. Keynote at HPCMASPA'23 Workshop.

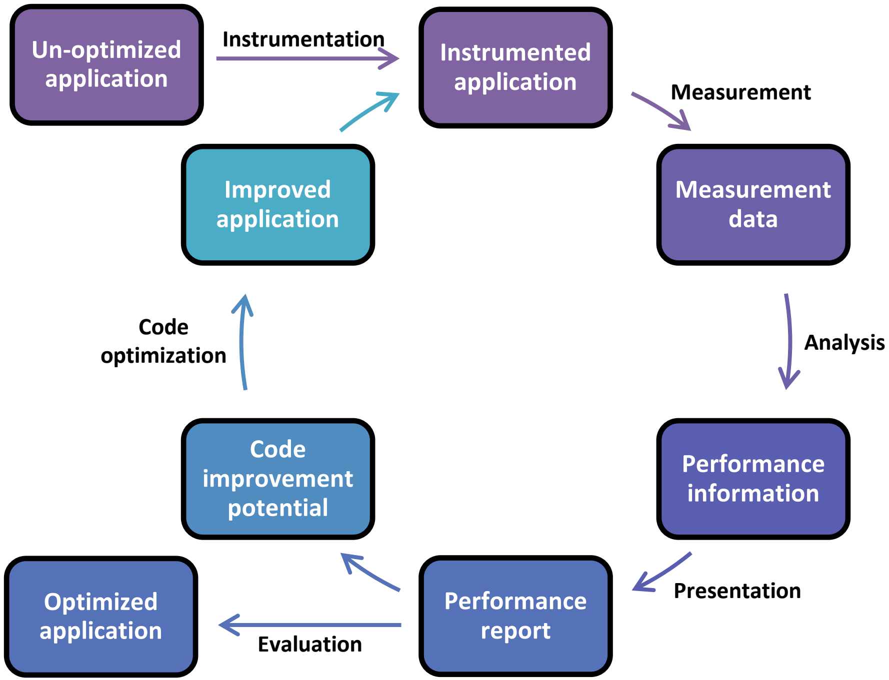
Dagstuhl Seminar 23171, 2023. *Driving HPC Operations With Holistic Monitoring and Operational Data Analytics*. https://www.dagstuhl.de/23171

# Diagnosing the Performance Trust Gap

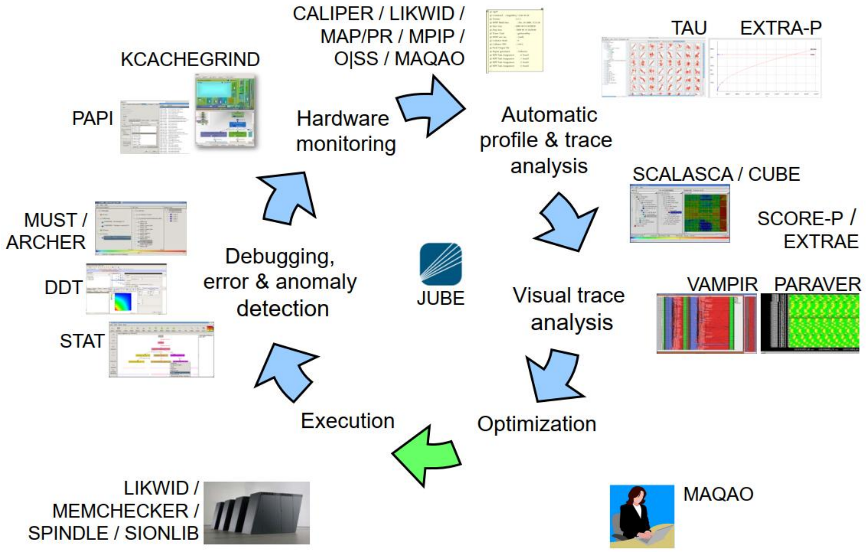
*Why current methods fall short*

# Diagnosing the Performance Trust Gap

## *The Traditional Performance Optimization Cycle*




### Example: Overview of the VI-HPS Tools

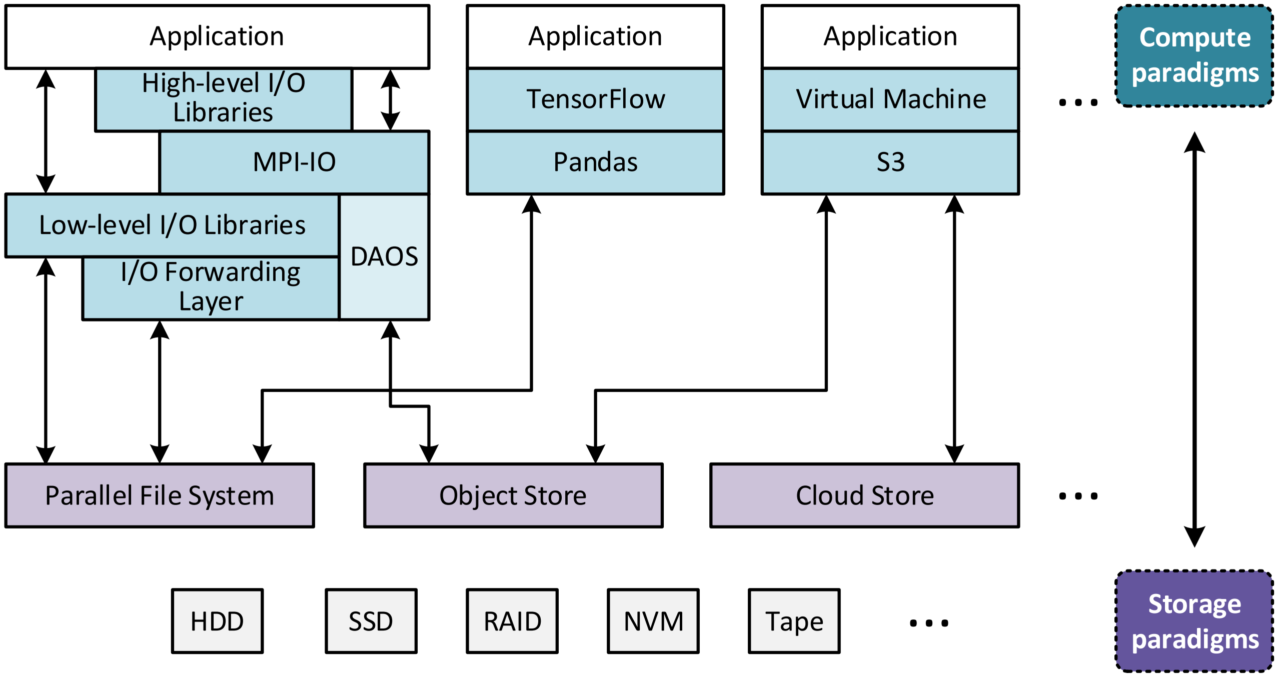



Performance Engineering Overview, https://doc.zih.tu-dresden.de/software/performance_engineering_overview/

Virtual Institute – High Productivity Supercomputing (VI-HPS), https://www.vi-hps.org/tools/tools.html

# Diagnosing the Performance Trust Gap

*Example: Parallel I/O Stack and its Performance Factors*




**Application**

- Number of processes
- Request sizes
- Access patterns
- I/O operation
- Data volume

**Network**

- Message sizes
- Network topology
- Network paths
- Network type

**File System**

- Type of file system
- Disk types
- Stripe sizes
- File hierarchy
- Shared access

# Diagnosing the Performance Trust Gap
*Example: Status of I/O Characterization Tools*

**Blue Waters, Mira, and Theta popular Darshan log sources used for research:**

- https://bluewaters.ncsa.illinois.edu/data-sets
- https://reports.alcf.anl.gov/data/
- ftp://ftp.mcs.anl.gov/pub/darshan/data

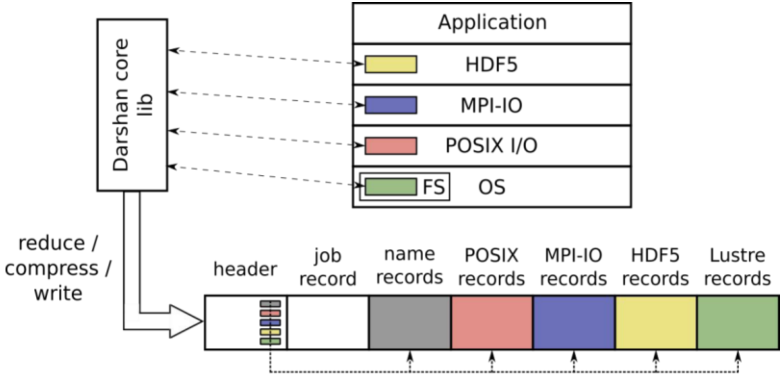
**Open questions:**

- How relevant are the logs to current systems?
- How do we know the integrity of the logs?

**Community comments:**

- "Darshan is one of the first tools to be deactivated in the event of I/O problems."
- "Darshan cannot grasp the complexity of state-of-the-art parallel storage systems."

**Darshan I/O Characterization Tool**




Snyder, S., 2022. *Darshan: Enabling Insights into HPC I/O Behavior*. ECP Community BoF Days.

**What are the implications of these questions and observations?**

# Diagnosing the Performance Trust Gap

## *Fragile Pipelines: Tool-Driven, Not Insight-Driven*

| Category | Examples | Srengths | Limitations |
|---|---|---|---|
| ***Application-level*** | Darshan, Recorder, Score-P | Fine-grained function tracing | No visibility into system-wide interactions |
| ***System-level*** | LDMS, DCDB, TACCStats | Aggregated I/O performance metrics | Cannot correlate application performance with system metrics |
| ***End-to-end*** | Ganglia, Nagios, Apollo | Holistic view of system utilization | Lacks deep profiling at kernel and network levels |

- **Siloed Tool Views:** *Each tool sees a layer. None explain the whole system.*
  => In case of I/O: App-level profilers (e.g., Darshan) vs. system tools (LDMS, DCDB)
- **Workflow Scripts Instead of Workflows:** *Custom scripts per experiment = unscalable, unrepeatable.*
  => Benchmarking tools (e.g., iperf, sockperf) often require client/server logic incompatible with SLURM
- **Discarded Insights:** *Performance data is ephemeral; models are not reused.*
  => No structure for reuse → repeated effort, lost opportunities

# Diagnosing the Performance Trust Gap

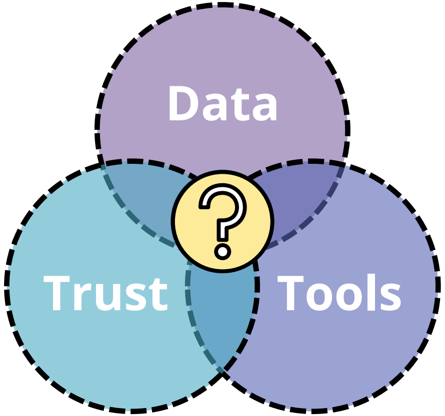
*Why We Need to Rethink HPC Performance Engineering*

- Heterogeneous Architectures
- Parallelism and Scalability
- Diversity of Workloads
- Dynamic Resource Allocation
- Software Stack Complexity
- Large-scale Data Movement
- Benchmark Suitability

Reproducibility

Portability

Comparability



# Reproducible, Tool-Agnostic Workflows for Performance Insight

*From ad hoc pipelines to robust, model-aware workflows*

# Reproducible, Tool-Agnostic Workflows

*Goal: Holistic & Automated Monitoring and Analysis Cycle*

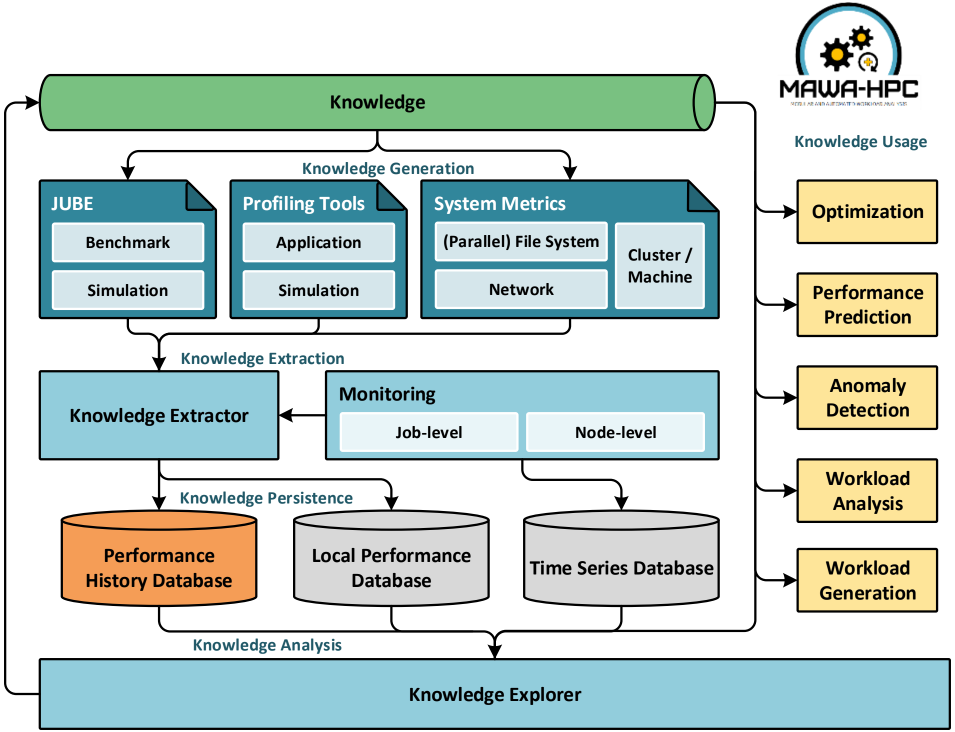
***Idea:*** Develop and implement standardized and tool-independent approach for HPC workload and application analysis

***Goal:*** Establish a ***performance history database*** to categorize systems, workload behaviors, and characteristic patterns for different science domains


Zhu, Z., Bartelheimer, N. and Neuwirth, S., 2023. *MAWA-HPC: Modular and Automated Workload Analysis for HPC Systems*. ISC'23.

Bartelheimer, N., Zhu, Z., and Neuwirth, S., 2023. *Toward a Modular Workflow for Network Performance Characterization*. IPDPSW'23.

Zhu, Z., and Neuwirth, S., 2023. *Characterization of Large-Scale HPC Workloads With Non-Naïve I/O Roofline Modeling and Scoring.* ICPADS'23.

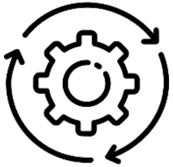



# Reproducible, Tool-Agnostic Workflows

*Reproducible Benchmarking and Measurement*

- ***Benchmarking:*** Process of comparing system performance using standardized tests and metrics.
- ***Reproducibility:*** Ability to obtain the same results with the same system and test conditions.
- ***Importance of Reproducibility:***
  - *Consistency:* Enables fair and accurate comparisons between systems
  - *Confidence:* Trust in benchmark results for decision-making
  - *Research Validity:* Essential for scientific studies and product evaluations


- ***Key Principles of Reproducible Benchmarking:***
  - *Documentation:* Record hardware and software configurations, test settings, and data
  - *Version Control:* Maintain consistent test suites and tools
  - *Automation:* Minimize human error by automating test execution
  - *Standardization:* Use industry-standard benchmarks and metrics
  - *Multiple Runs:* Conduct tests multiple times to verify results



# Reproducible, Tool-Agnostic Workflows

## *Reproducible Benchmarking: Integration is Key*

### Repeatability

- Ensures consistent results from the same setup
- Builds trust in computational outcomes
- Forms the basis for scientific validation

Schifrin, A., 2023. *Automated Performance Characterization of HPC Systems.* Bachelor thesis, Goethe University Frankfurt.

### Comparability

- Standardizes benchmarking across models or methods
- Allows fair evaluation of new approaches
- Helps identify performance trade-offs

Bartelheimer, N. and Neuwirth, S., 2023. *Toward Reproducible Benchmarking of PGAS and MPI Communication Schemes.* ICPADS'23.

### Modularity

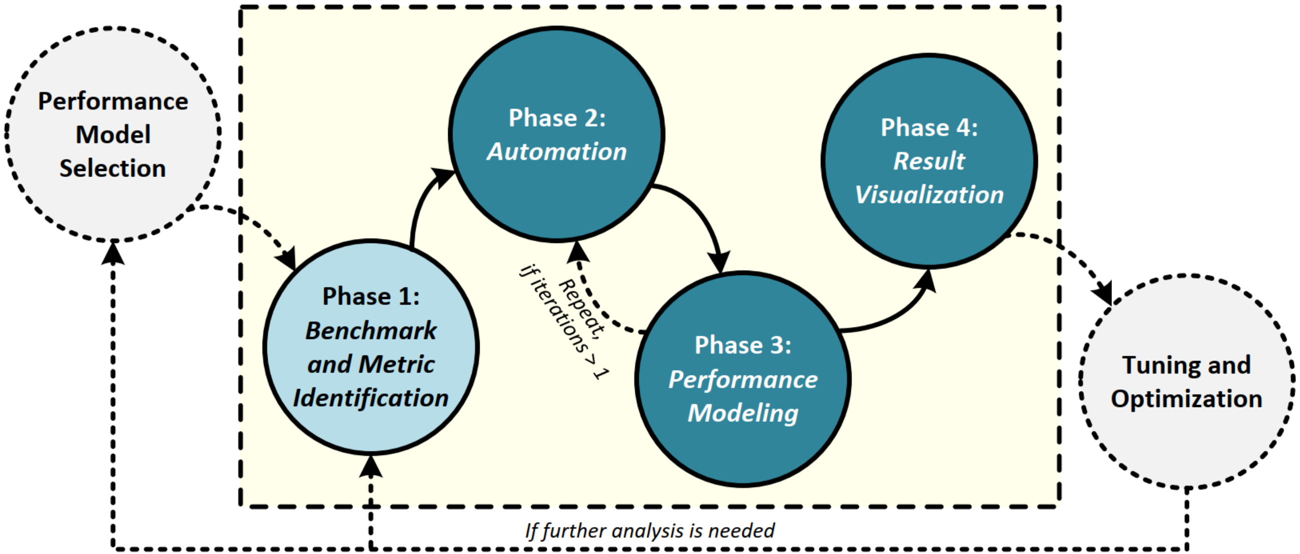
- Enables flexible software architecture
- Facilitates integration of AI/ML components
- Supports code reuse and maintainability

Zhu, Z., Wang, C. and Neuwirth, S., 2025. *Advancing HPC Performance Modeling with an Interactive, Automated and Tool-Agnostic ML-Driven Workflow*. SSDBM'25. (to appear)

# Reproducible, Tool-Agnostic Workflows

*Workflow Design for Reproducible Benchmarking*

Core component of the benchmarking framework is the **JUBE Benchmarking Environment**




```
config
├ platform
│ ├ fuchs
│ │ ├ platform.xml
│ │ └ platform-likwid-specs.xml
│ └ cesari
│   ├ platform.xml
│   └ ...
├ likwid-benchmark.xml
├ likwid-specs.xml
├ qperf-benchmark.xml
├ qperf-specs.xml
├ ...
├ likwid.run.in
└ ...
```

Bartelheimer, N., Zhu, Z., and Neuwirth, S., 2024. *Automated Network Performance Characterization for HPC Systems*. International Journal of Networking and Computing.

JUBE Documentation: [https://apps.fz-juelich.de/jsc/jube/jube2/docu/index.html](https://apps.fz-juelich.de/jsc/jube/jube2/docu/index.html)

# Reproducible, Tool-Agnostic Workflows

*Reproducible Benchmarking: Example Configuration*

**Benchmark-independent, Platform-specific**

`platform.xml`

```xml
<parameterset name="systemParameter">
    <parameter name="nodes" type="int">2</parameter>
    <parameter name="taskspernode" type="int">1</parameter>
    <parameter name="threadspertask" type="int">1</parameter>
    <parameter name="tasks" mode="python" type="int">$nodes * $taskspernode</parameter>
    <parameter name="timelimit">00:30:00</parameter>
</parameterset>
```

```xml
<parameterset name="executeset">
    <parameter name="submit">sbatch</parameter>
    <parameter name="submit_script">submit.job</parameter>
    <parameter name="starter">srun</parameter>
</parameterset>
```

**Benchmark-specific, Platform-independent**

`likwid-specs.xml`

```xml
<parameterset name="copy_params">
    <parameter name="benchmark_set_cp" tag="copy">        copy</parameter>
    <parameter name="benchmark_set_cp" tag="copy_avx">    copy_avx</parameter>
    <parameter name="benchmark_set_cp" tag="copy_avx512">copy_avx512</parameter>
</parameterset>
```

```xml
<parameterset name="alloc_params">
    <parameter name="alloc" tag="W">-W</parameter>
    <parameter name="alloc" tag="w">-w</parameter>
</parameterset>
```

```xml
<patternset name="likwid_pattern">
        <pattern name="likwid_cycles" type="int" dotall="False" mode="pattern">Cycles:\s+$jube_pat_int</pattern>
        <pattern name="likwid_cpu_clock" type="int" dotall="False" mode="pattern">CPU Clock:\s+$jube_pat_int</pattern>
</patternset>
```

**Benchmark-specific, Platform-specific**

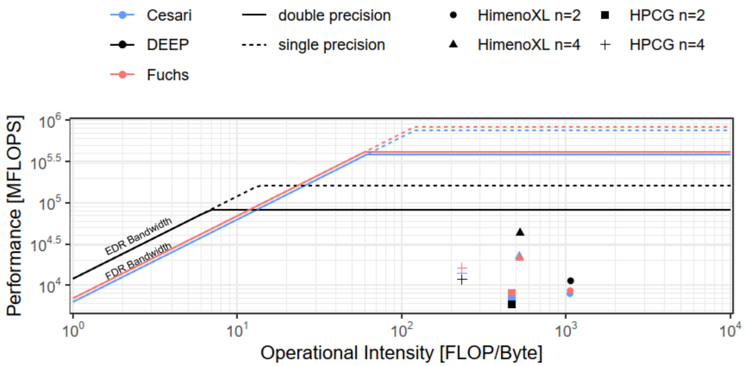
`platform-likwid-specs.xml`

```xml
<parameterset name="thread_domain_params">
    <parameter name="thread_domain" tag="td-n">  N</parameter>
    <parameter name="thread_domain" tag="td-s0">S0</parameter>
    <parameter name="thread_domain" tag="td-s1">S1</parameter>
    <parameter name="thread_domain" tag="td-d0">D0</parameter>
    <parameter name="thread_domain" tag="td-d1">D1</parameter>
    <parameter name="thread_domain" tag="td-c0">C0</parameter>
    <parameter name="thread_domain" tag="td-c1">C1</parameter>
    <parameter name="thread_domain" tag="td-m0">M0</parameter>
    <parameter name="thread_domain" tag="td-m1">M1</parameter>
</parameterset>
```

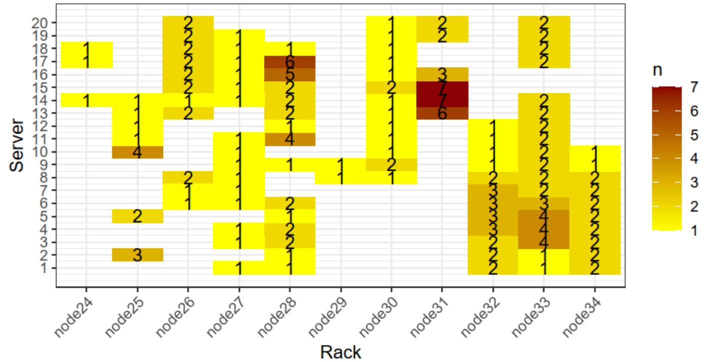
```xml
<parameterset name="suffix_params">
    <!--
        CHANGEME: this parameter can be changed and represents the parameter part after the <size>
        if not empty, the suffix must start with the ":" (colon) character
    -->
    <parameter name="suffix"></parameter>
</parameterset>
```

# Reproducible, Tool-Agnostic Workflows

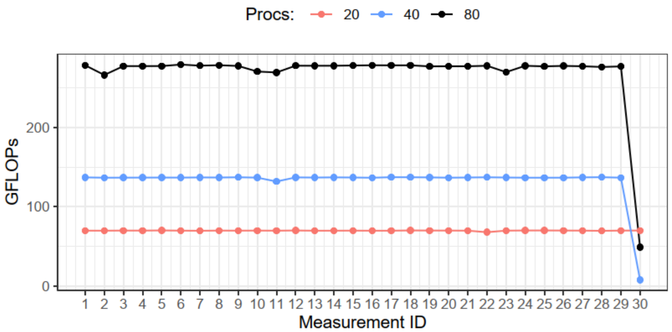
*Example: Automated Performance Characterization*



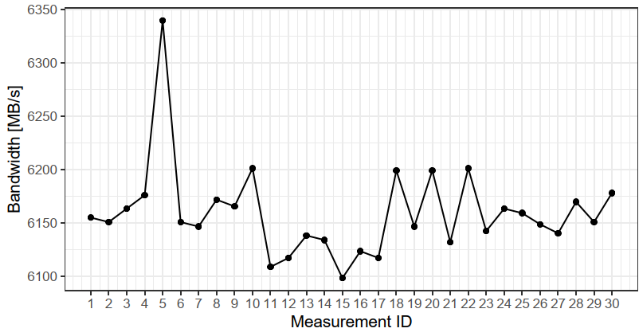

**Roofline model for Himeno and HPCG results.**




**Heat map of the allocated nodes (overall benchmark runs).**




**Himeno benchmark over 15 days / 2 measurements per day.**




**RDMA point-to-point performance over 15 days / 2 measurements per day.**

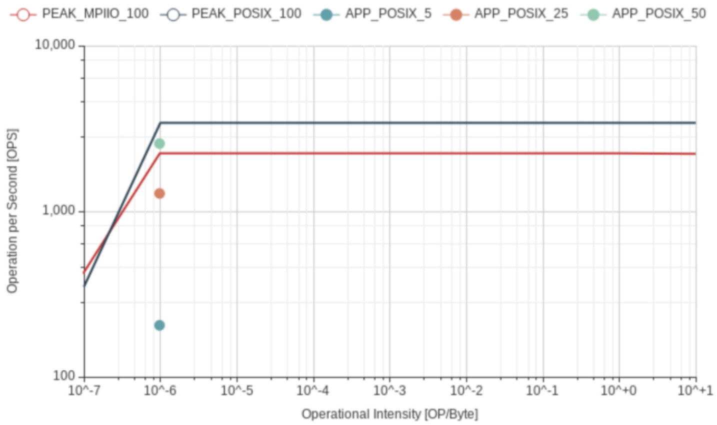
# Reproducible, Tool-Agnostic Workflows

## *I/O Roofline Characterization: Initial Concept*

Zhu, Z., Bartelheimer, N. and Neuwirth, S., 2023. *An Empirical Roofline Model for Extreme-Scale I/O Workload Analysis.* IPDPSW'23.

Zhu, Z., and Neuwirth, S., 2023. *Characterization of Large-Scale HPC Workloads With Non-Naïve I/O Roofline Modeling and Scoring.* ICPADS'23.

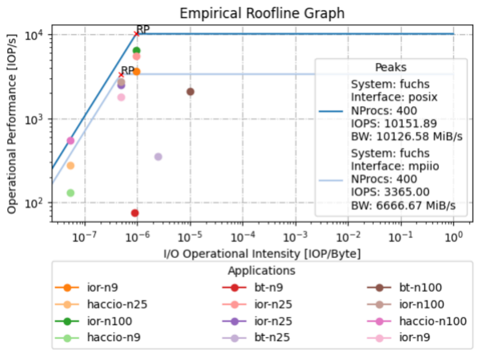
- Traditional Roofline Model…
  - is based on looking at the *relationship between work and traffic*
  - provides intuitive approach through simple bound and bottleneck analysis
- ***I/O Roofline Model*** is based on IOPS and the I/O bandwidth
  => *I/O interface specific*, i.e., POSIX, MPIIO, etc.
  - *IOPS*: number of reads and writes that a storage system can perform per second
  - *Bandwidth*: total amount of data read or written per second
- **X-axis:** *I/O Operational Intensity* $= \frac{\text{Total I/O Operations}}{\text{Read Bytes+Write Bytes}}$
- **Y-axis:** $P = \min(\text{Peak IOPS}, \text{Peak I/O Bandwidth} \times \text{I/O Intensity})$
  where $P$ is the attainable perf., $P_{peak}$ is the peak perf., $b$ is the peak bandwidth, and $I$ is the arithmetic intensity

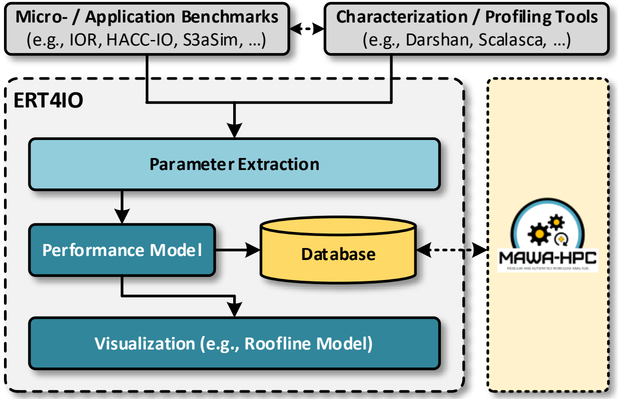


# Reproducible, Tool-Agnostic Workflows

## *I/O Roofline Characterization: Workflow Implementation*

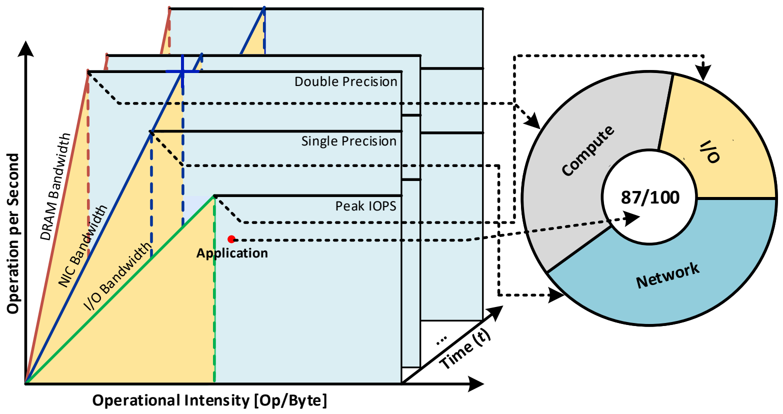
- *ERT4IO (Empirical Roofline Tool for I/O)* provides automated I/O Roofline characterization
  - Parameter extraction from Darshan logs
  - Generates Roofline visualization
- Forwards results to MAWA-HPC framework
  - Enables further data analysis
  - Preserves and shares knowledge via performance history database with the HPC community
- Applicable to various use cases
  - Systems with different configurations and hardware can be compared and evaluated
  - Intuitive estimation of an application's I/O performance
  - Identifying performance bottlenecks and anomalies



# Reproducible, Tool-Agnostic Workflows
## *Multi-dimensional Performance Modeling (WiP)*

- *Goal:* provide a comprehensive view of application and system performance ⇨ *emerging workloads*
- Multi-dimensional performance models, for example Roofline model, to account for multiple performance factors (e.g. network, compute power, and parallel I/O)
- Including time as an additional dimension, the Roofline model can provide insight into an application's performance over time, enabling the identification of performance anomalies

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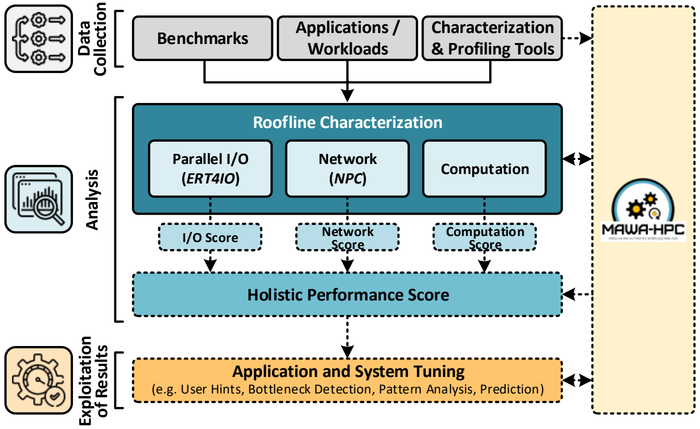
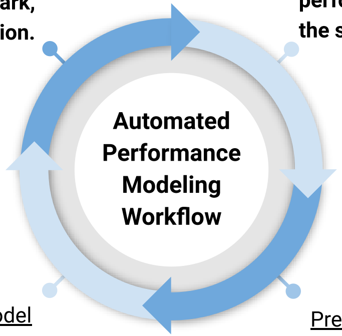


# Reproducible, Tool-Agnostic Workflows
## *Automated ML-Driven Performance Modeling Workflow*

Zhu, Z. and Neuwirth, S., 2024. *Interactive and Tool-Agnostic ML-Driven Workflow for Automated HPC Performance Modeling*. SC'24.

<u>Experiment Design</u>
**Design the experiment and set up the application, benchmark, or simulation.**

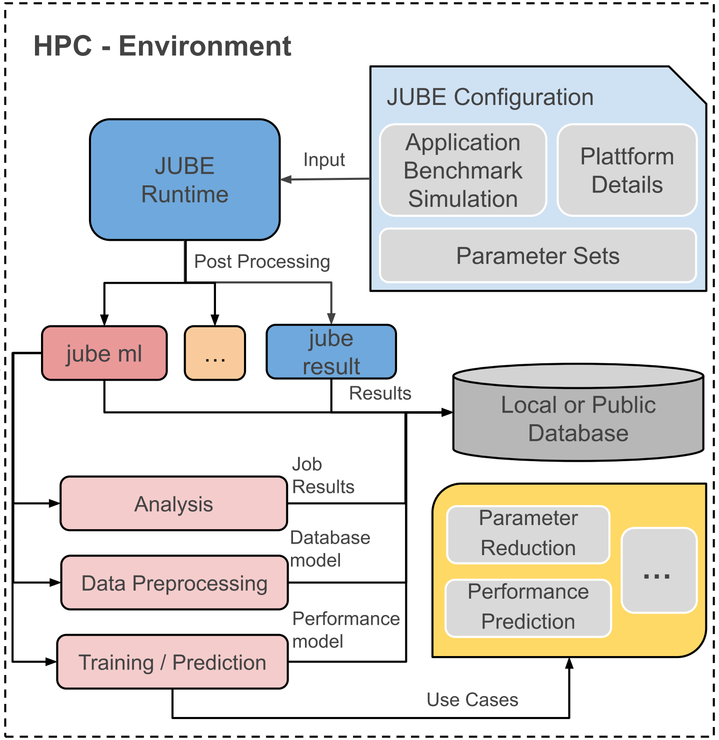
<u>Measurements</u>
**Run the experiment and collect and analyze performance results from the simulation.**




**Integration in JUBE**

<u>Create Performance Model</u>
**Split data into training and validation sets, train the model, validate it, and tune parameters until an acceptable model.**

<u>Pre Processing</u>
**Perform feature engineering and select the target. If necessary, clean the data.**

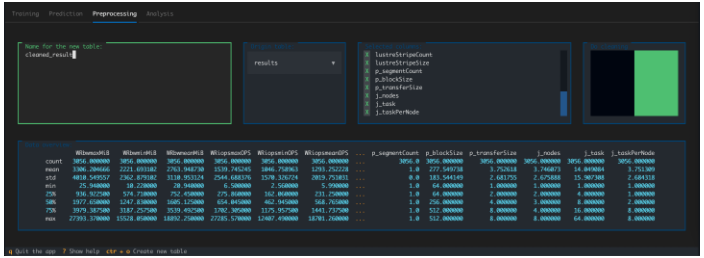



Zhu, Z., Wang, C. and Neuwirth, S., 2025. *Advancing HPC Performance Modeling with an Interactive, Automated and Tool-Agnostic ML-Driven Workflow*. SSDBM'25. (to appear)

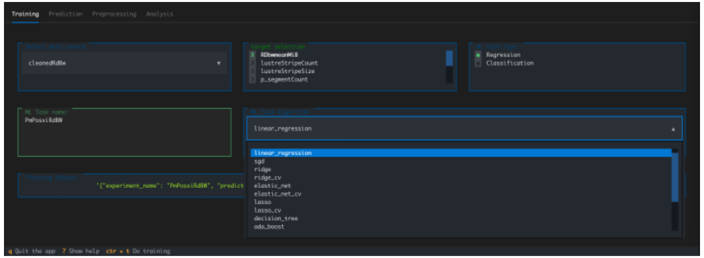
# Reproducible, Tool-Agnostic Workflows
## *JUBE-ML Prototype Implementation*

- Prototype *extends the JUBE framework* with support for automatic ML-based performance modeling and supports variety of ML algorithms
- JUBE-ML is enhanced by the *sqlite-ml extension*
- JUBE-ML stage provides *four key functionalities*:
  - ***Data analysis:*** insights into performance results (e.g., min, max, mean) and lambda functions
  - ***Data preprocessing:*** cleans and filters data for ML, creates new tables with selected features & targets
  - ***ML model training:*** applies ML models (regression or classification) to build a performance model
  - ***Prediction:*** validates the model & enables different analysis scenarios, such as identifying irrelevant parameters and predicting system performance

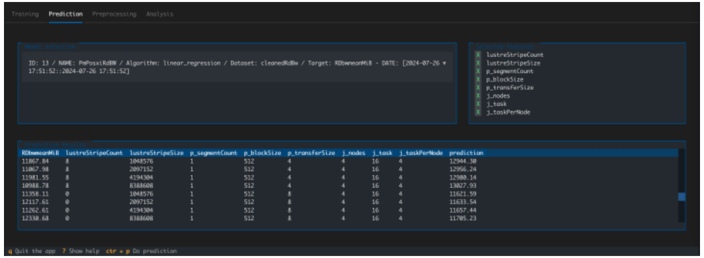
PRE-PROCESSING AND ANALYSIS



TRAINING PHASE



PREDICTION AND VALIDATION

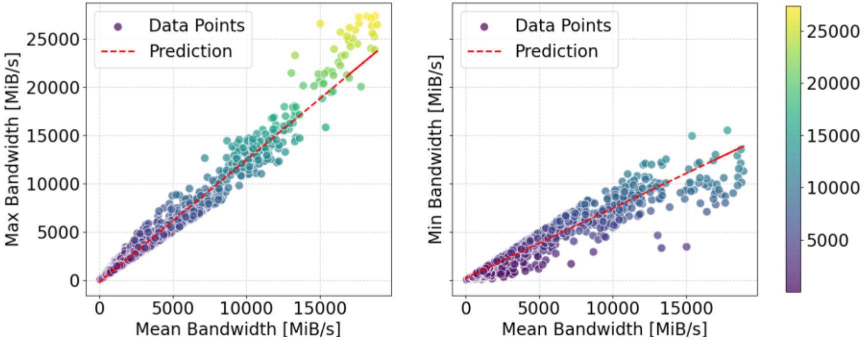


# Reproducible, Tool-Agnostic Workflows

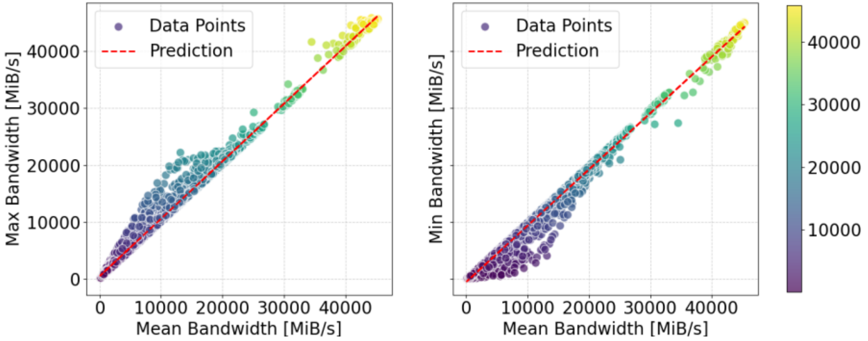
## *JUBE-ML Case Study: I/O Bandwidth*

- *Use Case:* I/O bandwidth modeling and prediction to demonstrate the JUBE-ML workflow
  - IOR benchmark to simulate various I/O workloads and generate performance data
  - Linear regression: 25% for training, 75% for validation
- Despite the small training sample, the model predicts both minimum & maximum bandwidths well

| | |
|---|---|
| Block size | 64MB, 256MB, 512MB |
| Transfer size | 1MB, 2MB, 4MB, 8MB |
| Lustre striping count | 0, 2, 4, 8 |
| Lustre striping size | 1MB, 2MB, 4MB, 8MB |
| Nodes | 1, 2, 4, 8 |
| Tasks per node | 1, 2, 4, 8 |




**POSIX write performance prediction with JUBE-ML.**




**POSIX read performance prediction with JUBE-ML.**

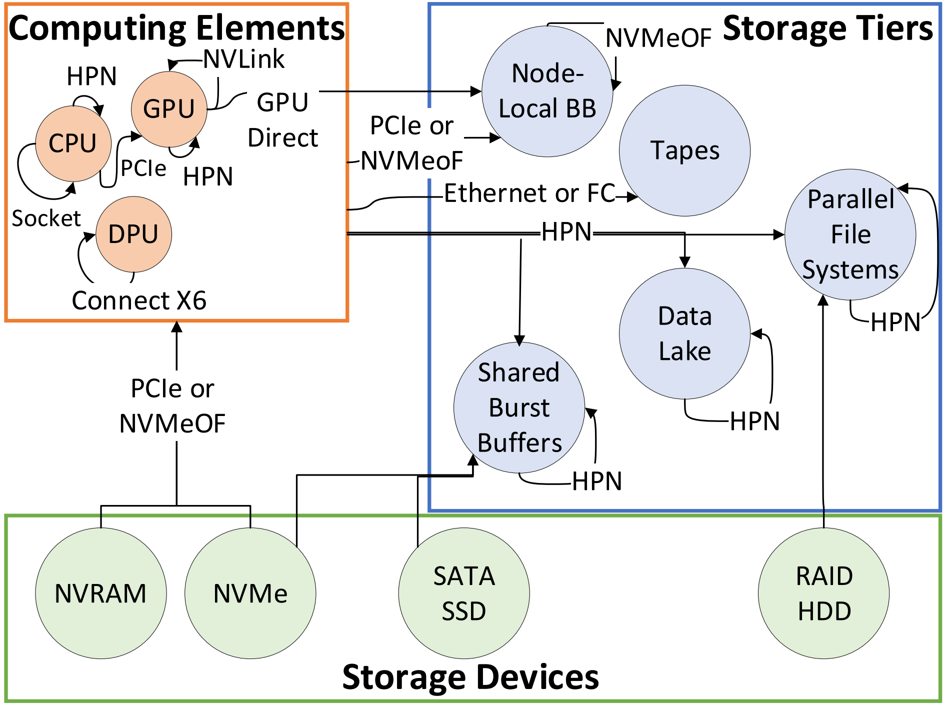
# Toward Explainable and Verified HPC Performance

*Bridging measurement and meaning through explainable models and verified traces*

# Toward Explainable and Verified HPC Performance

## *Master Architectural Plan (MAP)*

- Derived from current TOP500 and IO500
- Comprehensive framework designed to encapsulate the evolution of HPC storage architectures
- Primary objective of MAP is to provide a ***standardized yet adaptable blueprint*** to align software and monitoring tools across various HPC configurations
- ***Graph-based representation*** of components and interconnects for modeling data flows in HPC systems

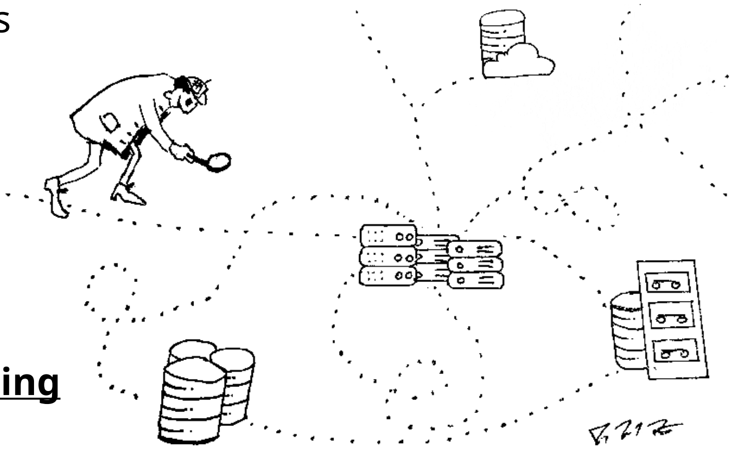



Neuwirth, S. and Devarajan, H., Wang, C., and Lofstead, J.., 2025. *XIO: Toward eXplainable I/O for HPC Systems*. SSDBM'25. (to appear)

# Toward Explainable and Verified HPC Performance

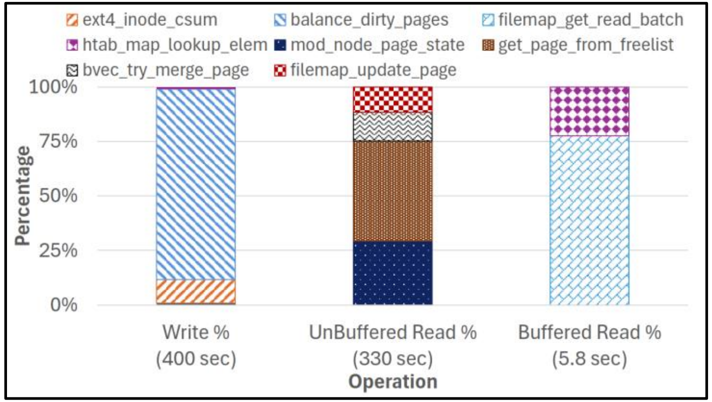
## *DataCrumbs: Comprehensive I/O Profiling*

- Only a few paths are covered by user-space monitoring tools
- Need access to more levels of software stack:
  - Multi-level software stack for high-level libraries
  - Multi-level kernel stack to understand buffering and stack cost
  - Multi-component to understand communication used for data movements
- **<u>DataCrumbs Approach: Low-Overhead Multi-Layer Profiling</u>**
  - Lightweight tool using eBPF (or SystemTap)
  - Attaching probes to user applications, middleware & kernel components => enabling transparent monitoring of relevant information
  - Sampling aggregated kernel data at configurable intervals => I/O patterns, buffer states, and system interactions
  - Correlating I/O function calls with kernel stack events, exposing bottlenecks such as page cache inefficiencies, metadata overhead, and system call latencies

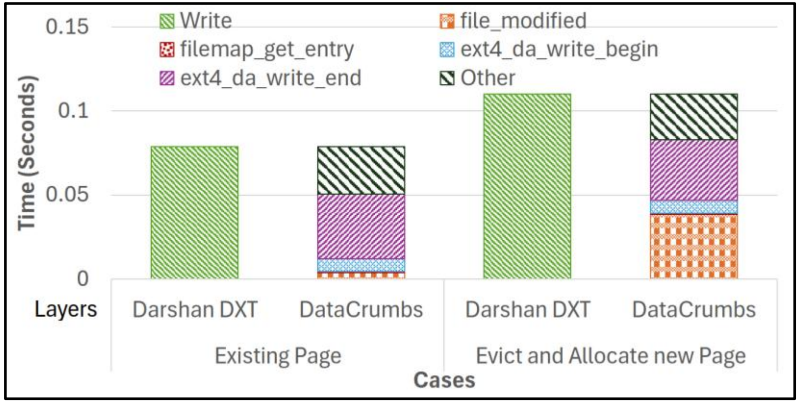


# Toward Explainable and Verified HPC Performance

## *Initial Evaluation: DataCrumbs vs. Darshan DXT*




**Performance breakdown with DataCrumbs for different read and write operations.**



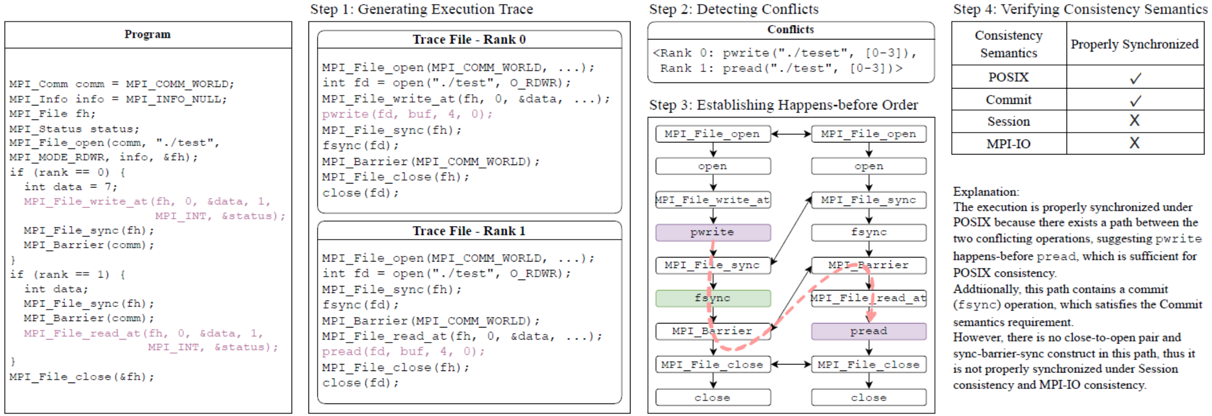

**Comparison of IOR performance breakdown with DataCrumbs and Darshan for two use cases.**

- ***Write operations (POSIX I/O):*** 82% of execution time spent on OS page cache management, highlighting impact of dirty page flushing
- ***Unbuffered read operations:*** High overhead due to frequent page cache misses
- ***Buffered read operations*** use different kernel functions
- ***Comparison of DataCrumbs and Darshan*** highlights need for visibility within kernel file system stack to understand performance variability within applications

Neuwirth, S. and Devarajan, H., Wang, C., and Lofstead, J.., 2025. *XIO: Toward eXplainable I/O for HPC Systems*. SSDBM'25. (to appear)

# Toward Explainable and Verified HPC Performance

*VerifyIO: Verifying Parallel I/O Consistency Semantics*

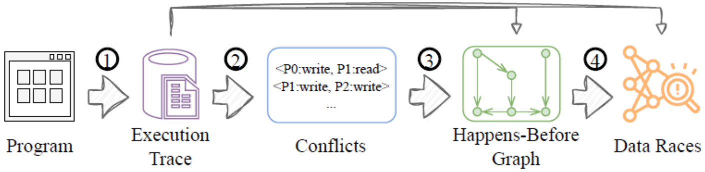



**Goals:**

- ***Ensure correctness*** on relaxed consistency systems
- ***Diagnose portability issues*** across backends
- ***Support future file systems*** beyond POSIX
- ***Enable developers*** to detect and fix semantic violations

**What is VerifyIO?** An open-source tool for trace-based verification of I/O consistency semantics in HPC applications.

**Why does it matter?** Emerging file systems and libraries relax consistency models (e.g., MPI-IO, Session), which can silently break application correctness.




Wang, C., Zhu, Z., Mohror, K., Neuwirth, S., and Snir, M., 2025. *VerifyIO: Verifying Adherence to Parallel I/O Consistency Semantics*. IPDPS'25. (to appear)

# Toward Explainable and Verified HPC Performance
## *FlexBench: From Traces to Tunable I/O Benchmarks*

**FlexBench is…**
- A benchmark generator that reconstructs and manipulates I/O patterns from execution traces
- Built on top of Recorder+, leveraging Context-Free Grammars (CFGs) to compress and describe I/O behavior

**Why do we need FlexBench?**
- Traditional tracing tools like Darshan or Recorder capture detailed I/O but lack replay and what-if capabilities
- FlexBench enables users to replay, analyze, and tune the I/O behavior of applications, even without modifying code

**Core Goals:**
1. Use CFGs to precisely describe application I/O patterns
2. Reproduce original I/O performance from filtered traces
3. Expose optimization opportunities (e.g., parameter tuning)

**Step 1: Recording the Full Trace**

**Step 2: Filtering for a Clean Trace**

**Step 3: Deriving the Benchmark**

**Step 4: Performance Optimization**

# Conclusions

# Conclusions

*Open Problems and Community Challenges*

## Benchmarking Trust

- What does it mean to trust a performance result?
- Can we quantify trust the way we quantify performance?

## Metadata Standardization

- Can we converge on trace metadata schemas across tools?
- How do we ensure trace context is captured and preserved?

## From Metrics to Meaning

- What constitutes a verified insight?
- Can we establish common ground between correctness verification and performance validation?

## Reproducibility at Scale

- How do we scale reproducibility beyond case studies?
- What community infrastructure (e.g. shared testbeds, curated traces) do we need?

**Trustworthy performance insights are sustainable insights.**

# Thank you for your Attention!

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