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## Introduction

### Underpredictions

- Early job terminations
- Reduced system efficiency

### Overpredictions

- Increased job waiting time
- Idle resources

Users **manually** request

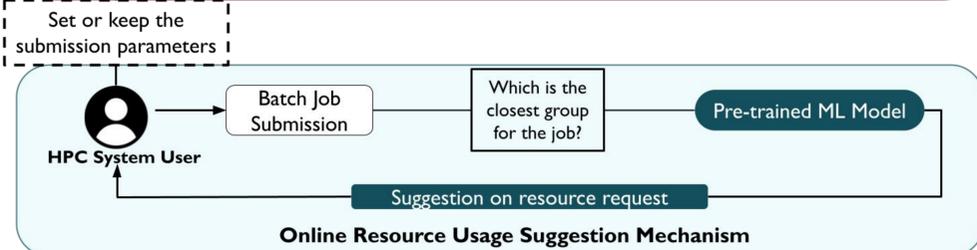
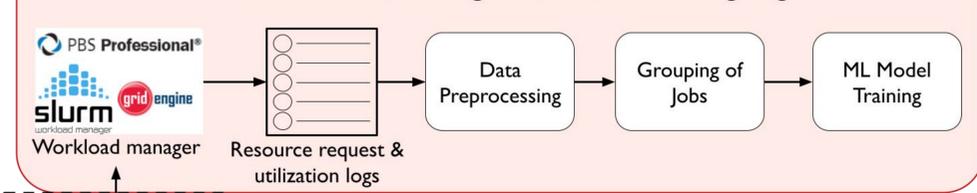
- Execution Time
- Number of Processors
- Maximum Memory Size
- Compute Nodes

### Goals:

- Predict HPC batch jobs resources to limit under and overpredictions
- Provide resource recommendations to HPC system users
- Increase overall system utilization and QoS, reduce resource waste

## Objectives & Framework Design

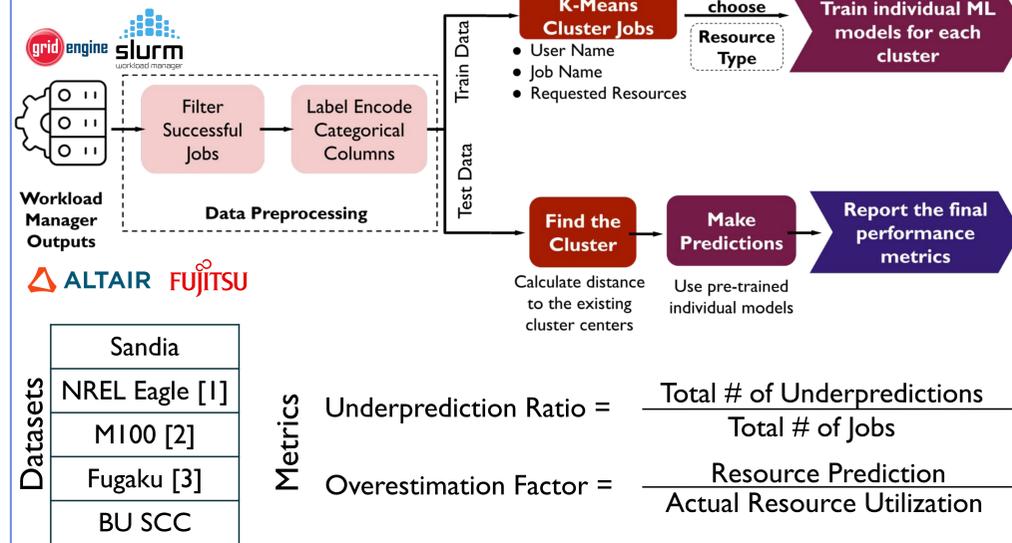
### Offline Machine Learning Based Predictor Training Stage



- Model training and testing inputs: batch job submission parameters – such as user, job and project name and requested resources
- Applying data driven strategies after model training to prevent the underestimation of resources

↓ User Wait Time    ↑ Job Throughput    ↓ CPU Node Hours

## Experimental Methodology



ALTAIR FUJITSU

Sandia
NREL Eagle [1]
M100 [2]
Fugaku [3]
BU SCC

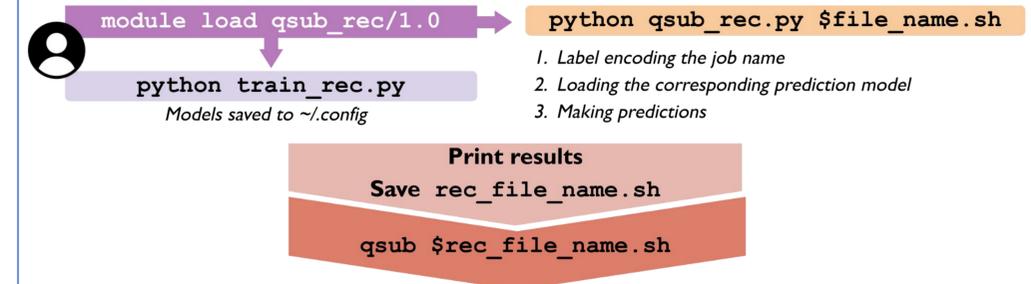
Datasets

Metrics

$$\text{Underprediction Ratio} = \frac{\text{Total \# of Underpredictions}}{\text{Total \# of Jobs}}$$

$$\text{Overestimation Factor} = \frac{\text{Resource Prediction}}{\text{Actual Resource Utilization}}$$

## Real System Deployment



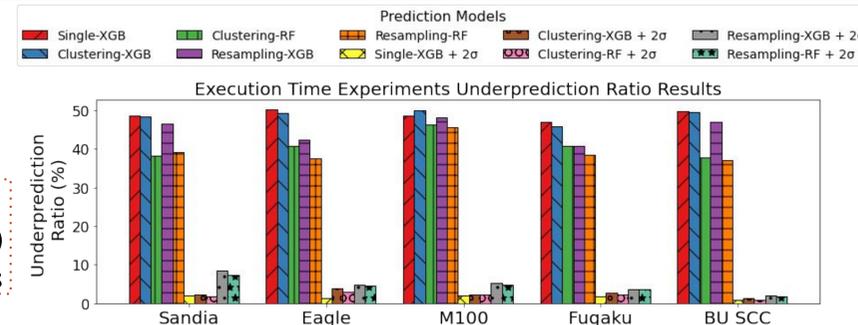
- **Goal:** Provide **online**, data-driven resource request suggestions before jobs are queued
  - An Lmod [4] environment module for Boston University Shared Computing Cluster (BU SCC) users
- Aiming to reduce wait times and resource waste while increasing efficiency and job throughput on BU SCC

## Results

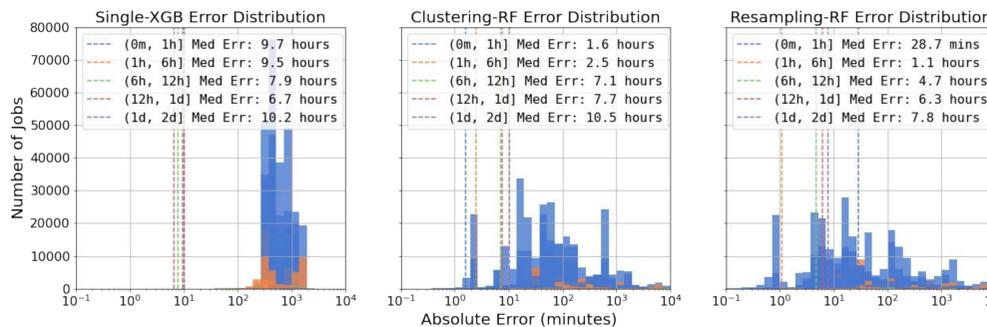
### Offline inference experiments

Baseline: Menear et al. [1] XGBoost model

Resampling Changing the training dataset distribution  
Buffering Adding an offset ( $2\sigma$ ) to model predictions



Execution Time Absolute Error Results on Eagle Dataset (with 2σ buffer)



Reducing underprediction ratio of target resource variables to less than 2% and limiting overpredictions.

## Conclusion & Future Work

- Job clustering + smaller models results in lower MAE and outperforms the baseline method
- Towards real-time recommendations to users

- Future work:
  - Test on a production HPC system with real batch jobs
  - Analyze resource usage variance
  - Explore dynamic resource management solutions

### References:

[1] Menear, K., Nag, A., Perr-Sauer, J., Lunacek, M., Potter, K., & Duplyakin, D. (2023). Mastering HPC runtime prediction: From observing patterns to a methodological approach. Practice and Experience in Advanced Research Computing 2023: Computing for the Common Good (PEARC '23), 75–85. Association for Computing Machinery.  
 [2] Borghesi, A., Di Santi, C., Molan, M., et al. (2023). M100 ExaData: A data collection campaign on the CINECA's Marconi100 Tier-0 supercomputer. Scientific Data, 10, 288.  
 [3] Antici, F., Bartolini, A., Domke, J., Kiziltan, Z., & Yamamoto, K. (2024). F-DATA: A Fugaku Workload Dataset for Job-centric Predictive Modelling in HPC Systems (1.0) [Data set]. Zenodo.  
 [4] McLay, Robert, et al. "Best practices for the deployment and management of production HPC clusters." State of the Practice Reports. 2011. 1-11.

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