Ergonomics and efficiency of workflows on HPC clusters

Jakub Beránek

Supervisor
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Thesis goal

Design approches for executing workflows
on HPC clusters in an easy & efficient way

Thesis objectives

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1. Identify HPC workflow challenges

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2. Design approaches for overcoming them

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3. Implement them in a task runtime

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3. Implement them in a task runtime
4. Analyze results on real use-cases

Ergonomics and efficiency
of **workflows on HPC clusters**

Workflows

= task graphs, pipelines, task DAGs*, …

* Directed Acyclic Graph

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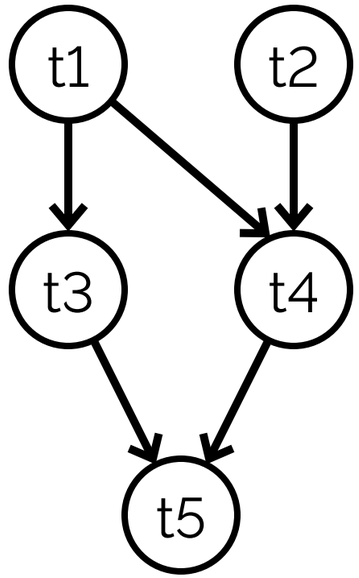
Popular programming model



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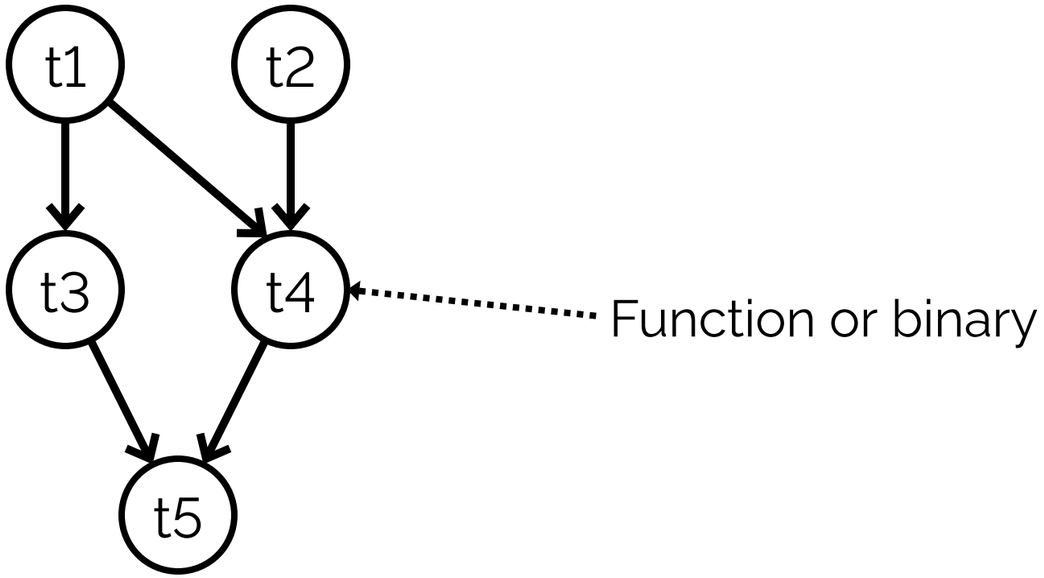

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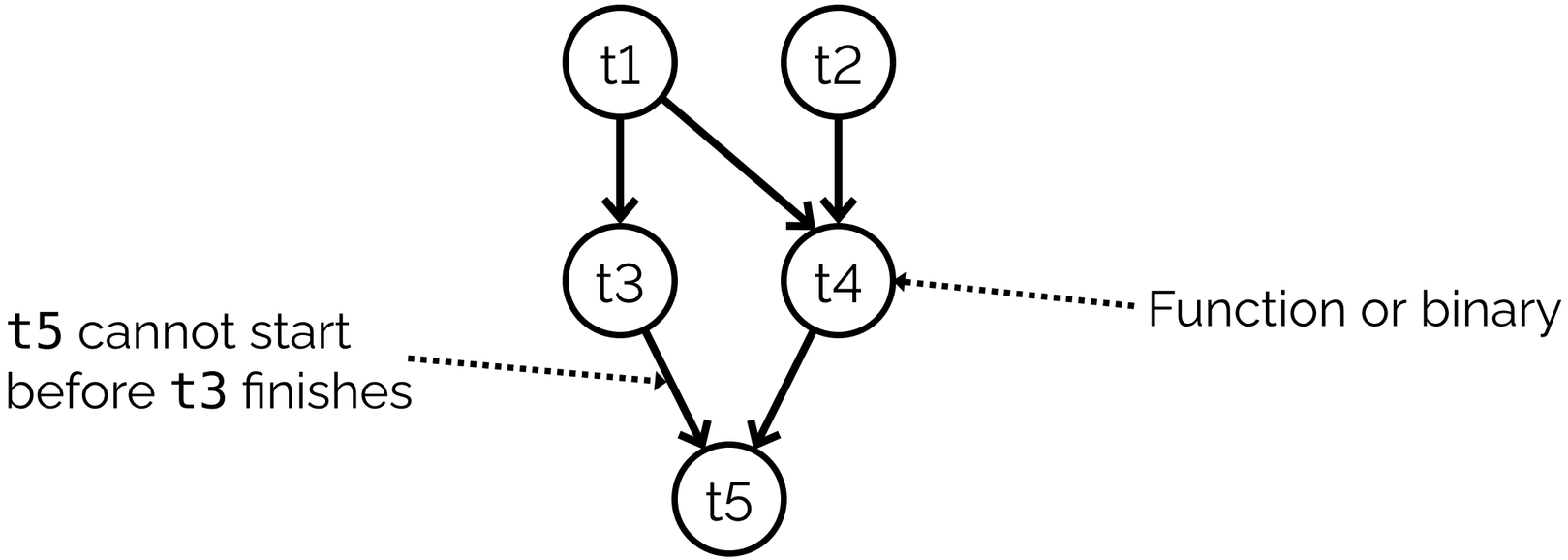

* Directed Acyclic Graph

Benefits of task-based programming

- **Implicit parallelism**
  - Create a DAG vs. explicit MPI calls
  - Extracted by a task runtime

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  - Extracted by a task runtime
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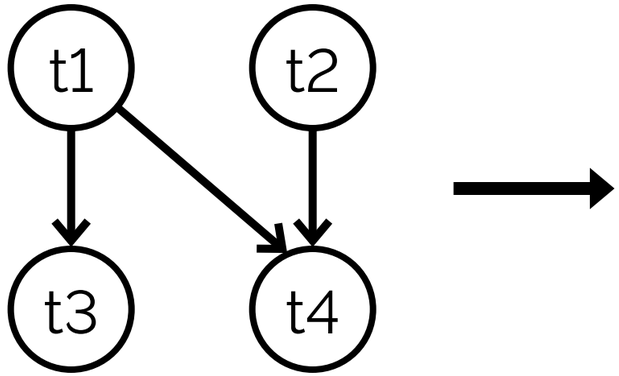
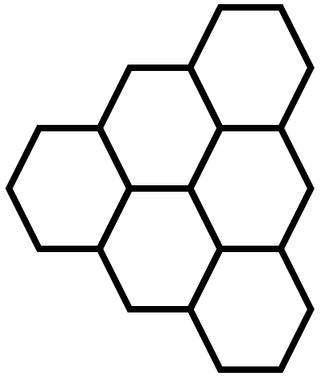
  - Python/DSL vs. C/C++
- Portability

Workflow challenges on HPC clusters

Allocation manager





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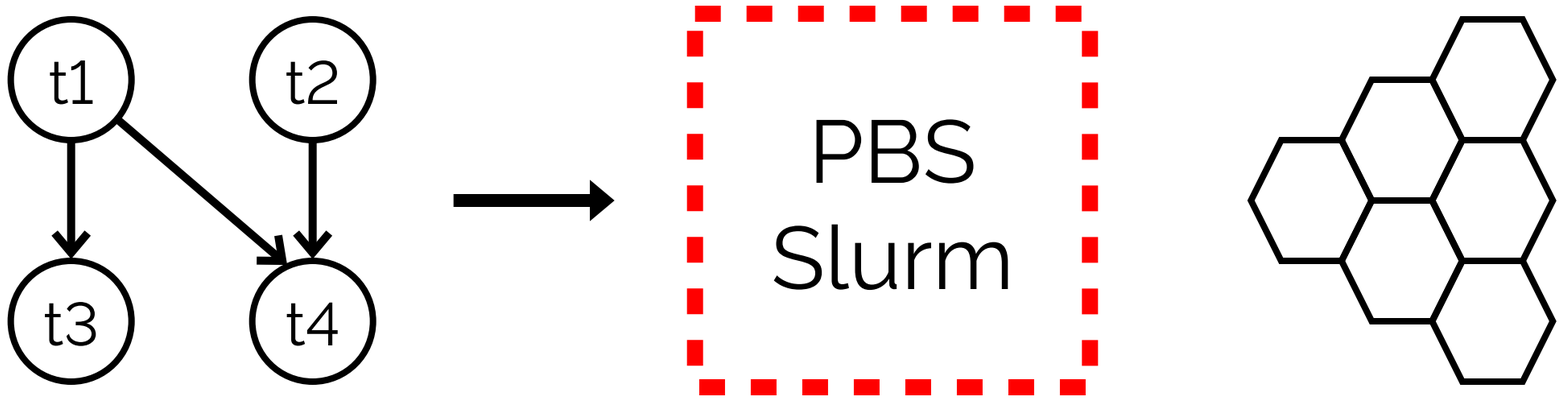
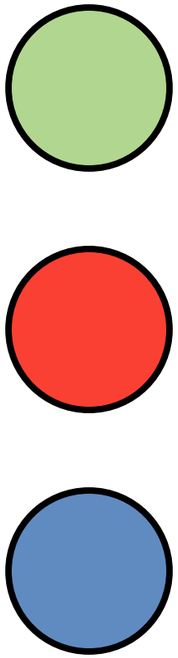
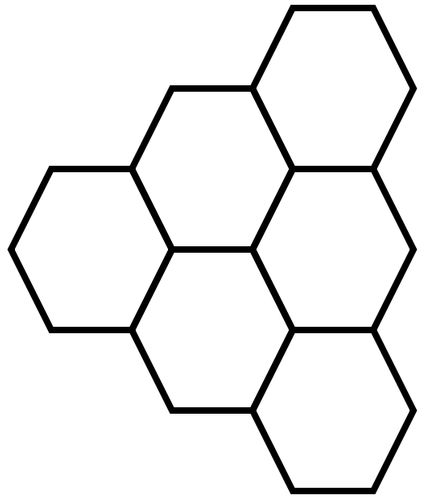


A few large tasks ✅





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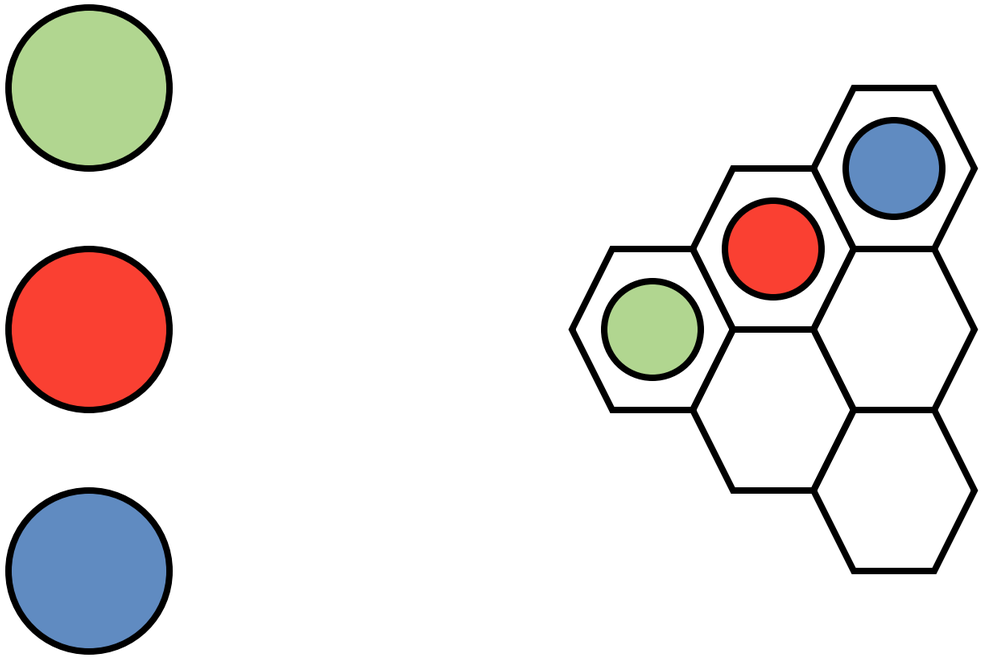
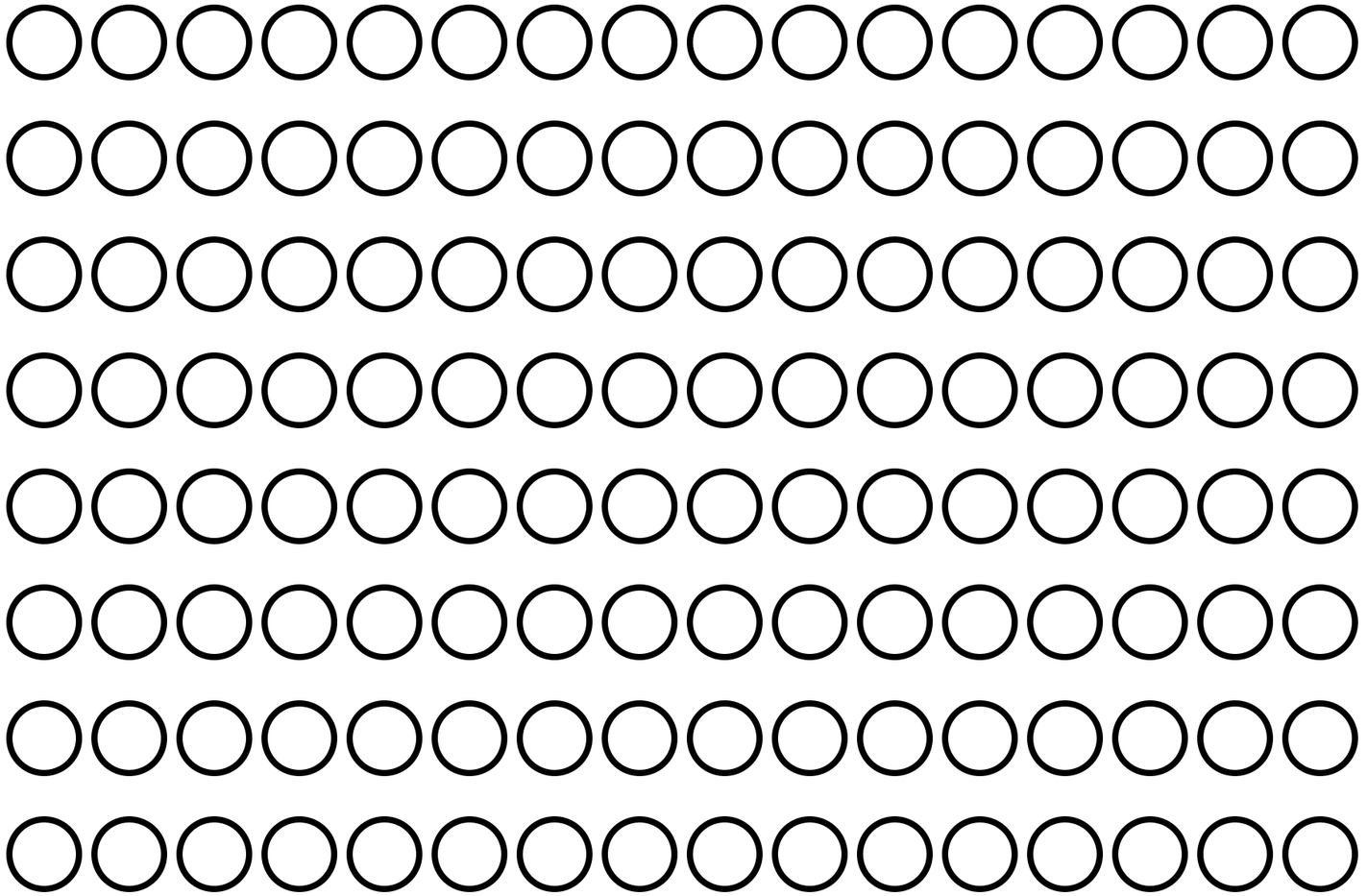


Many tasks



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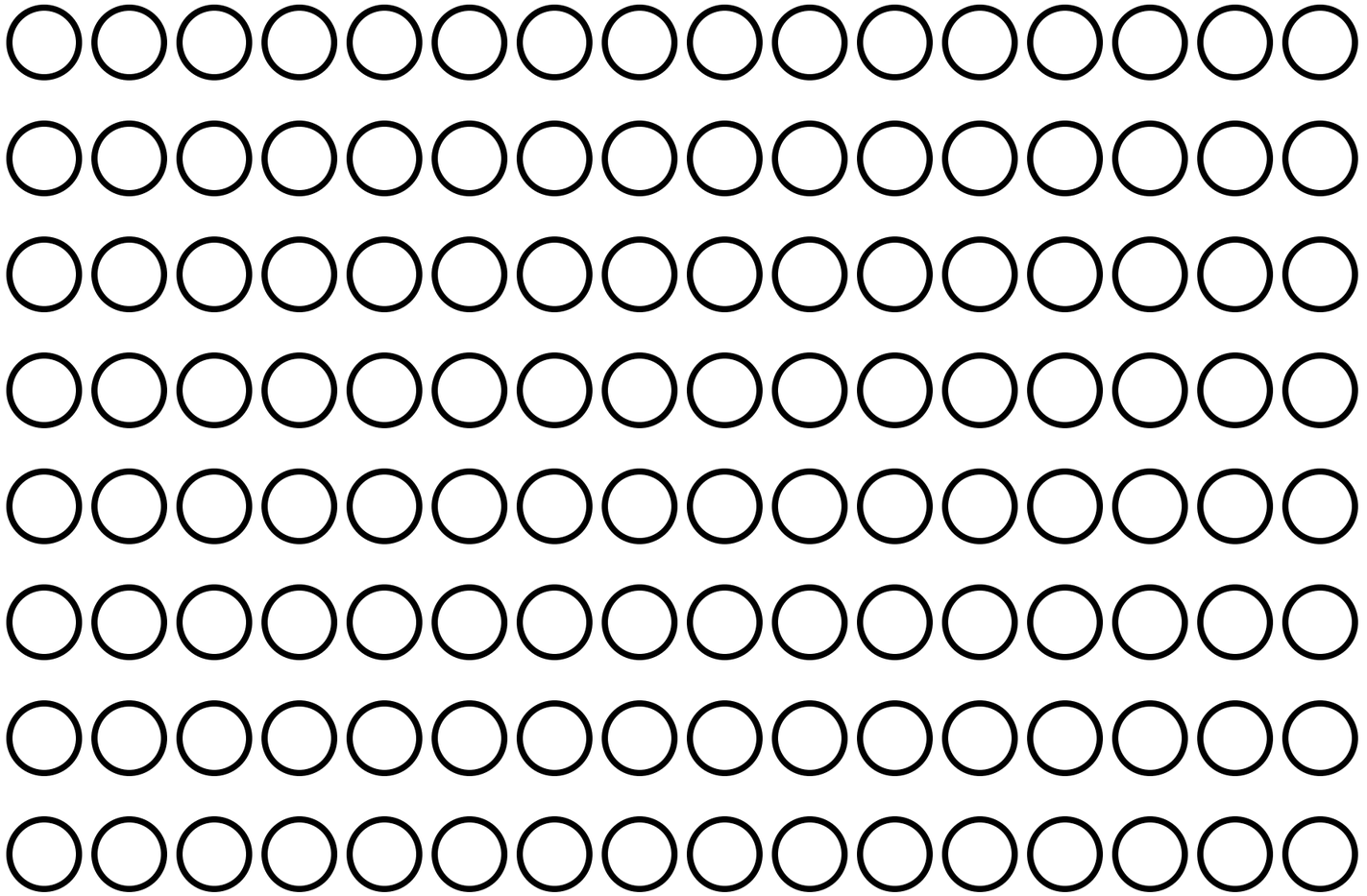

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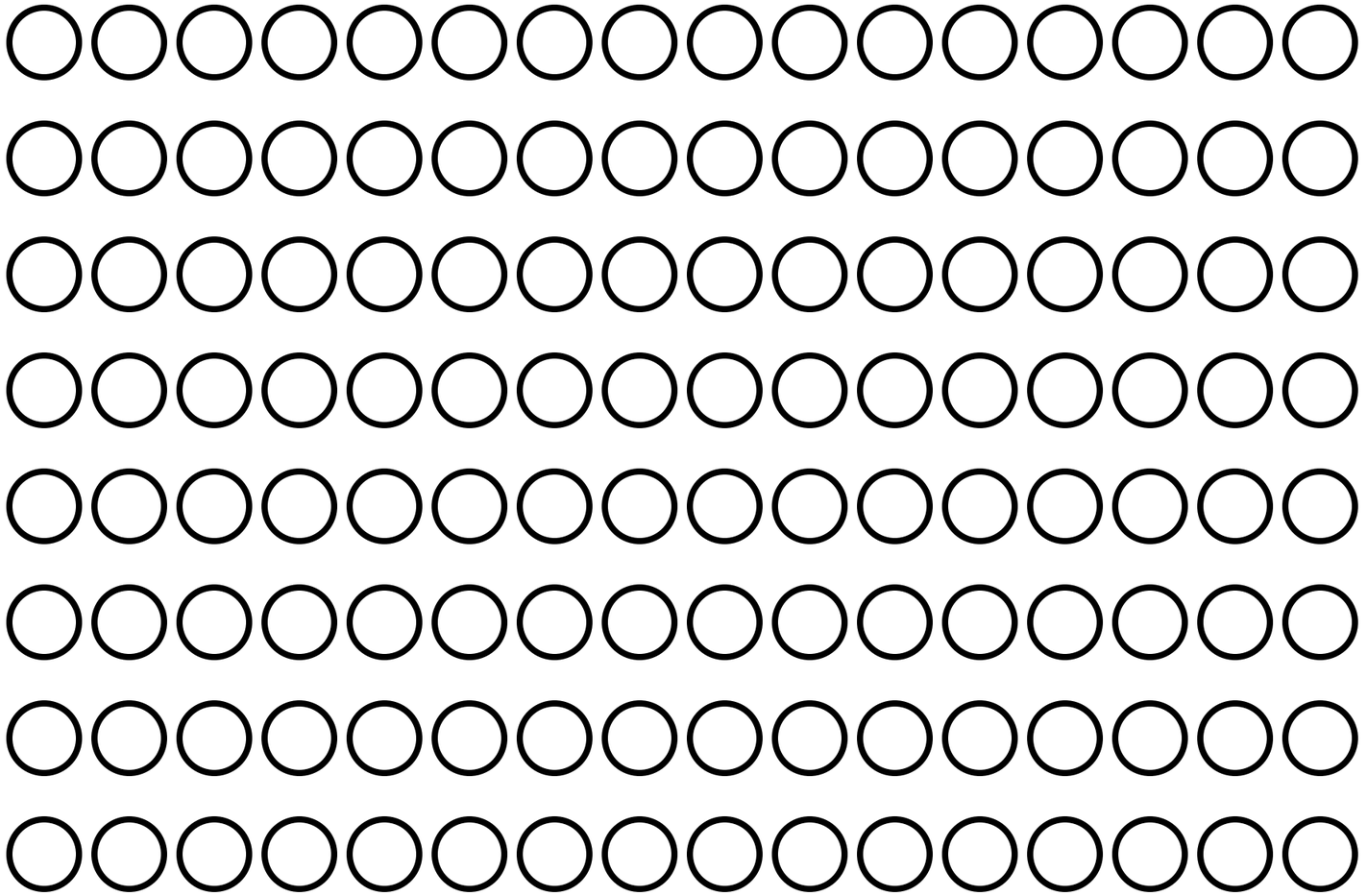

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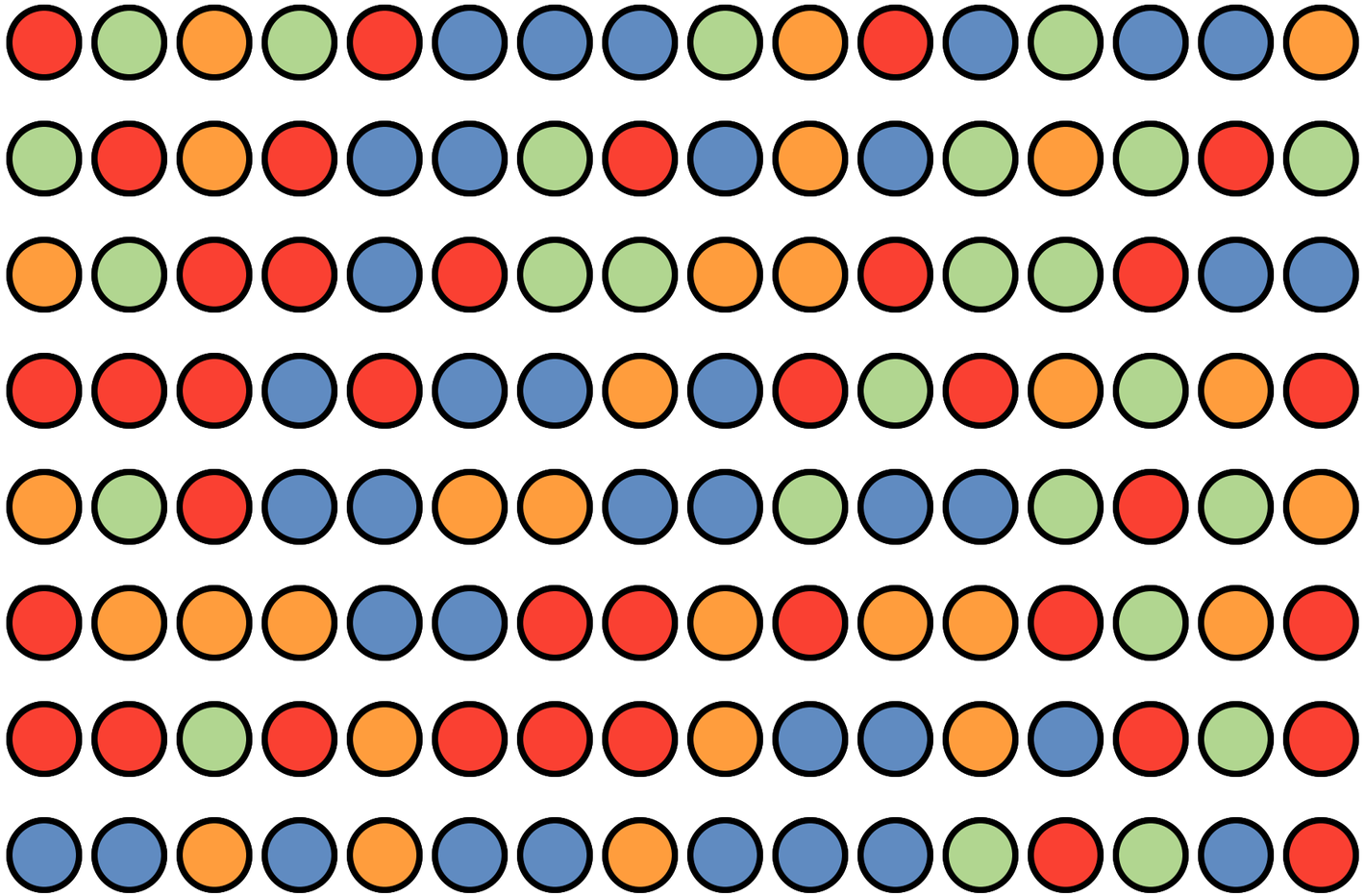
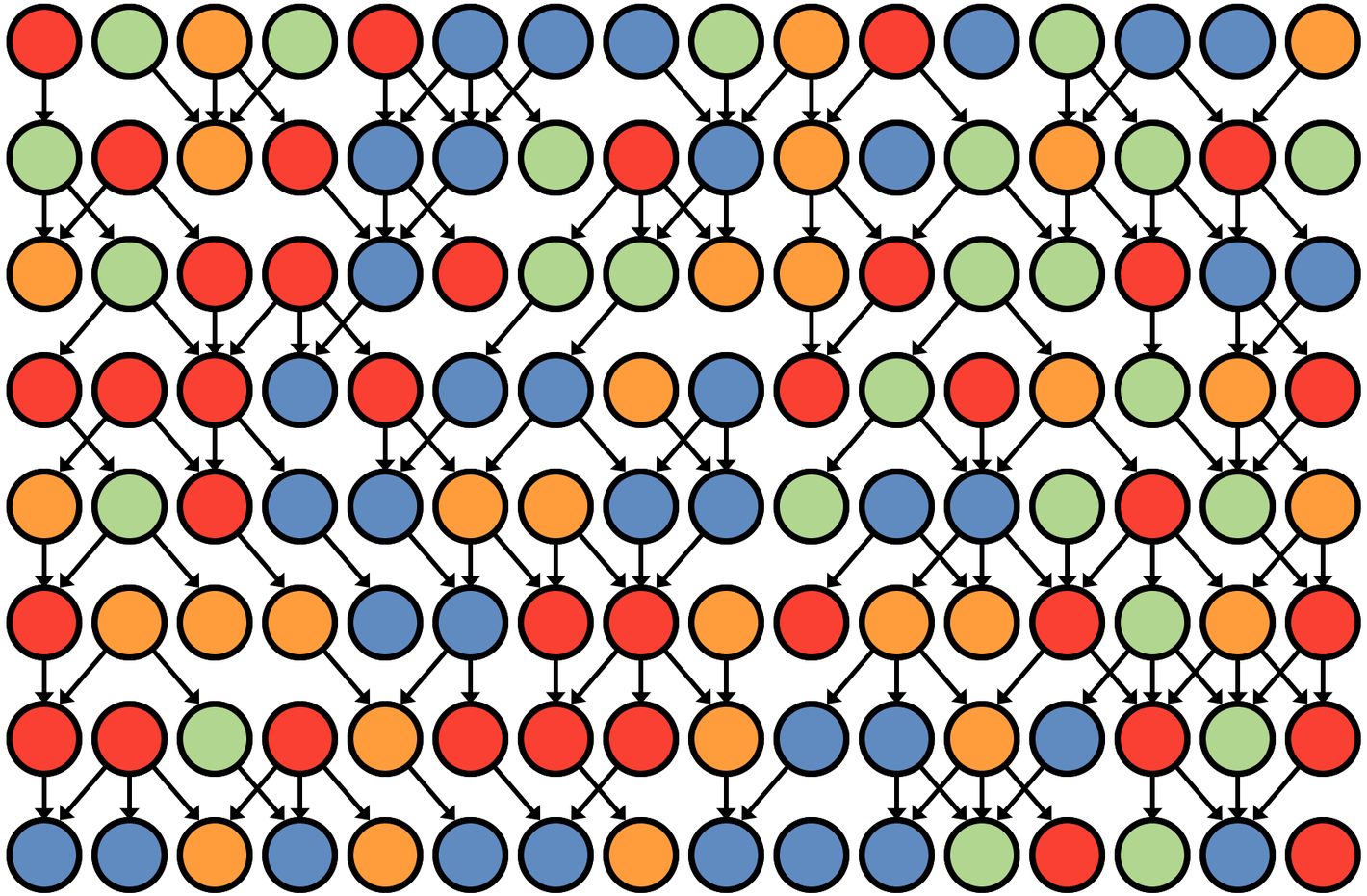
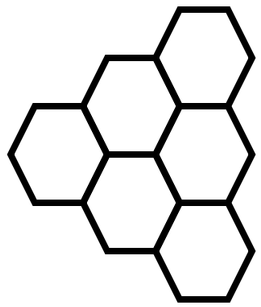


Task dependencies



Heterogeneous clusters



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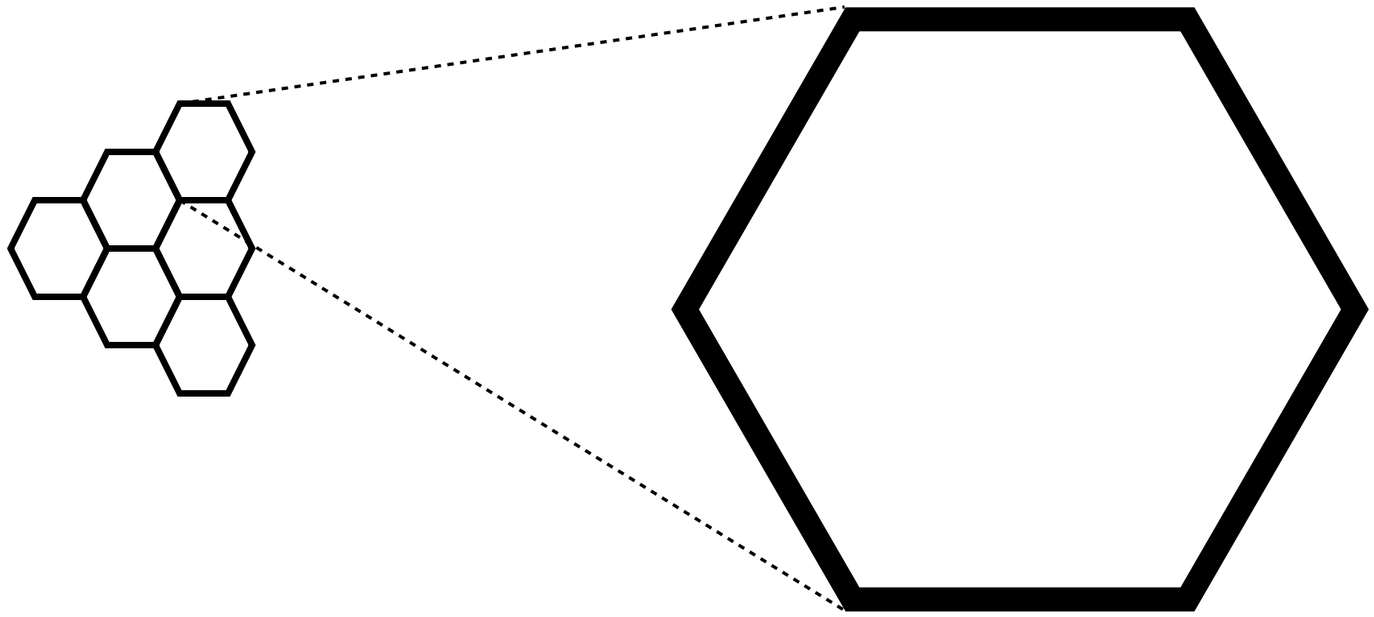

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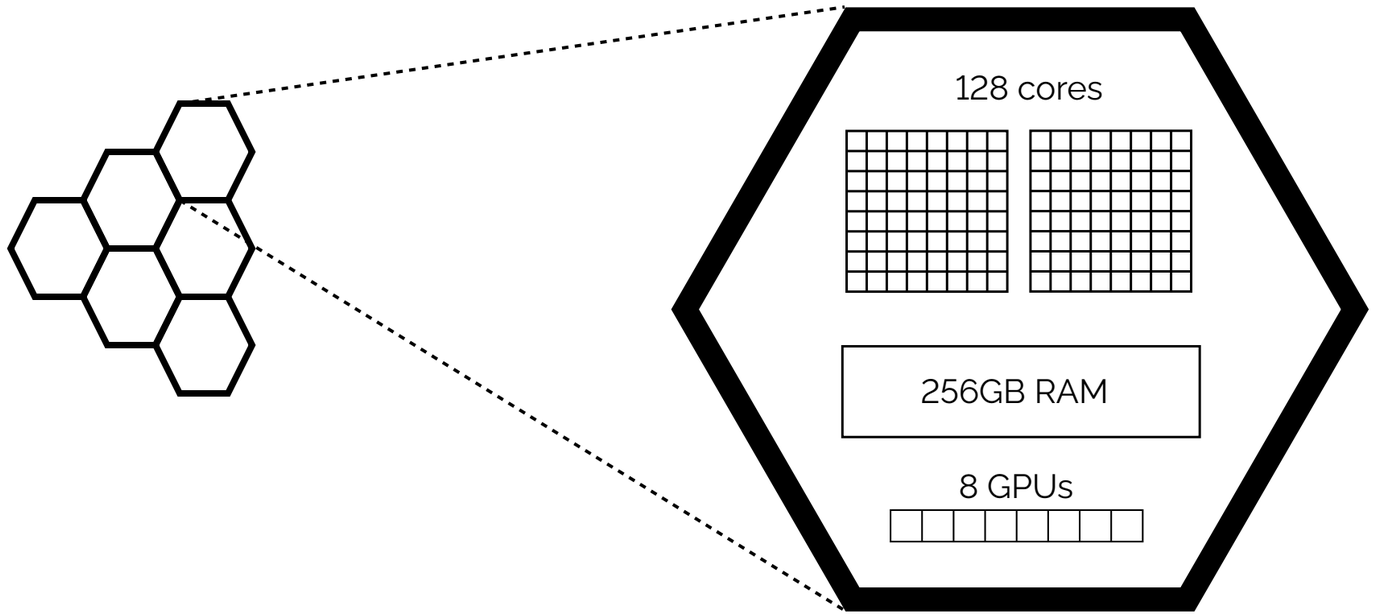

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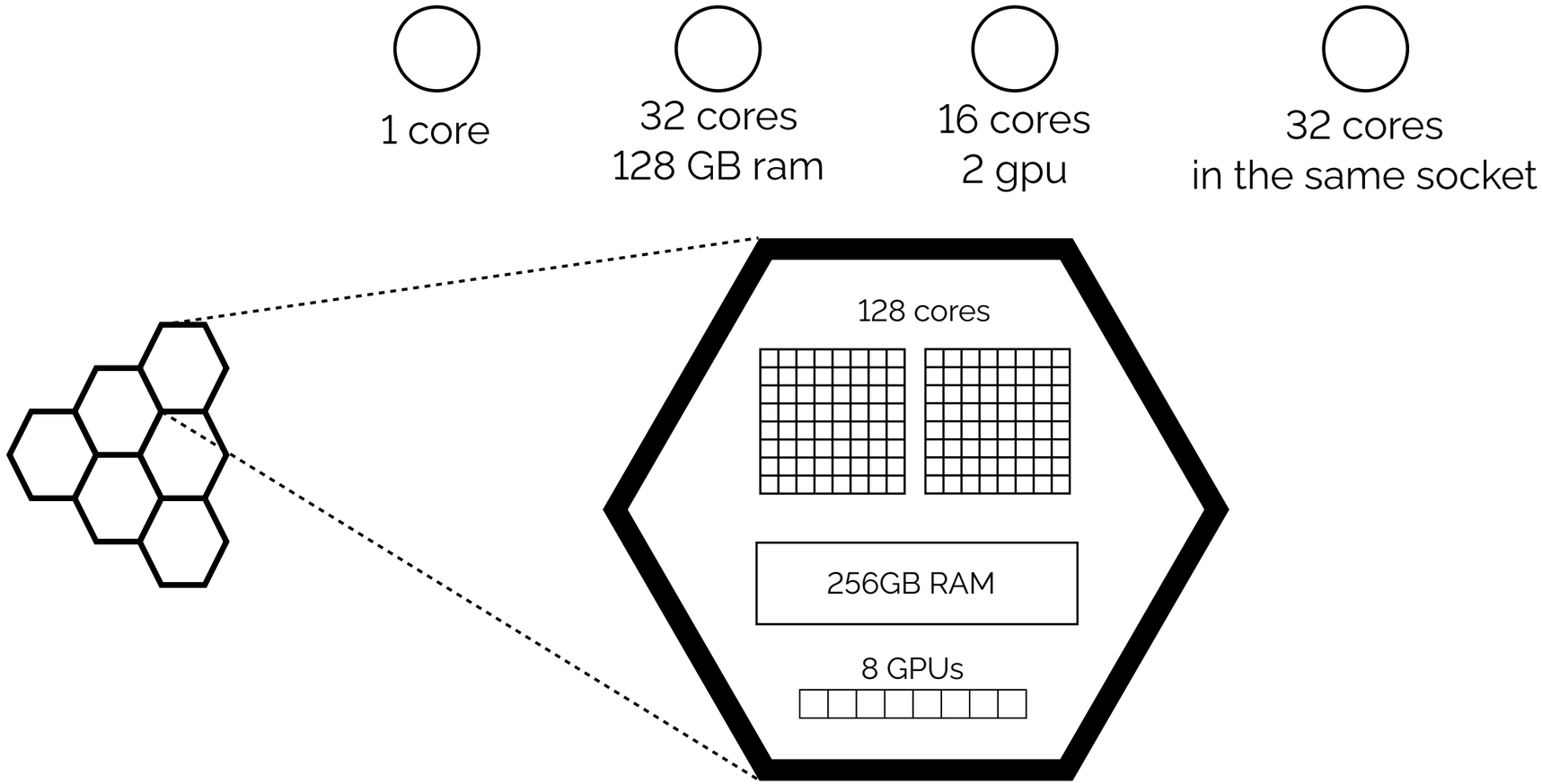

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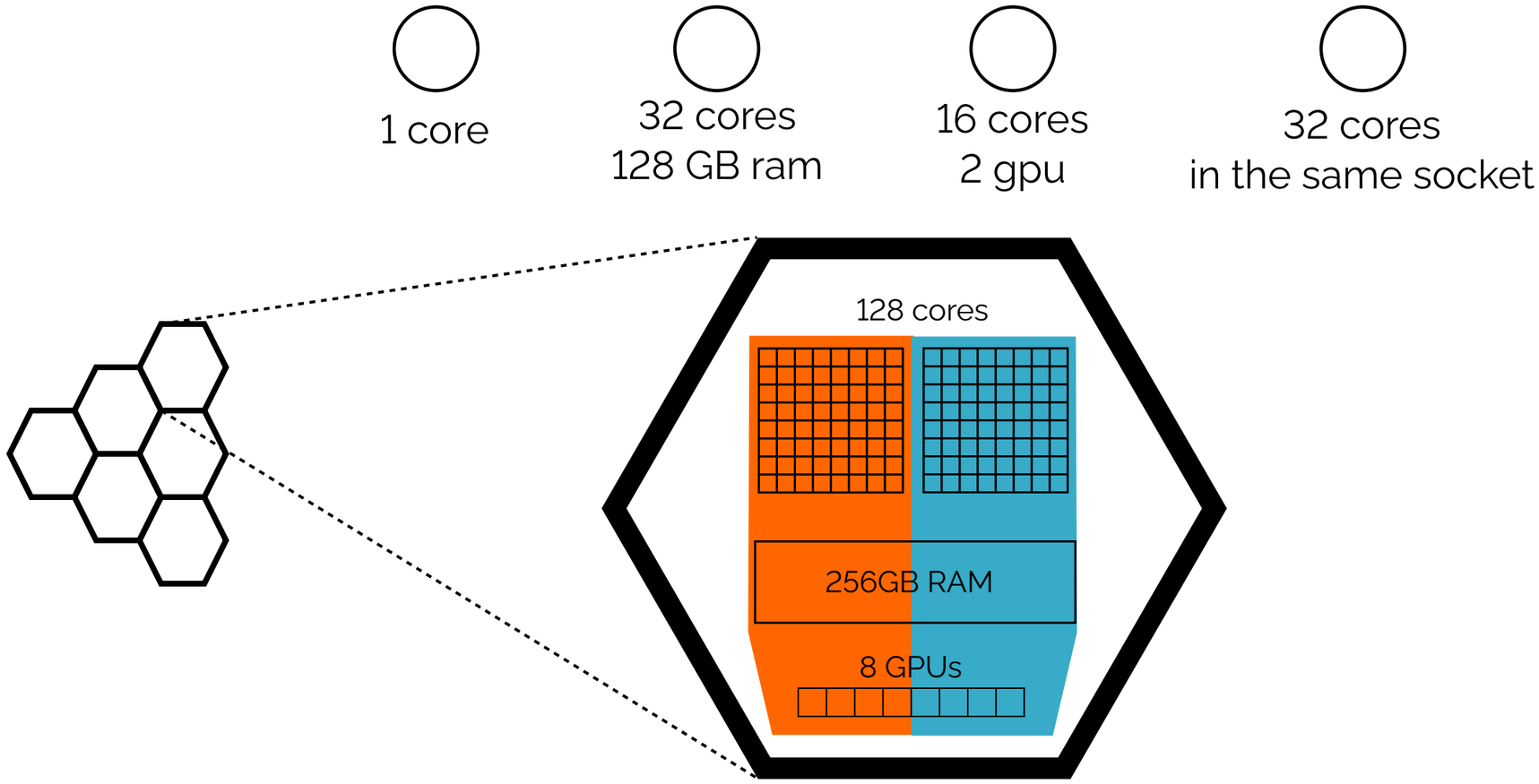

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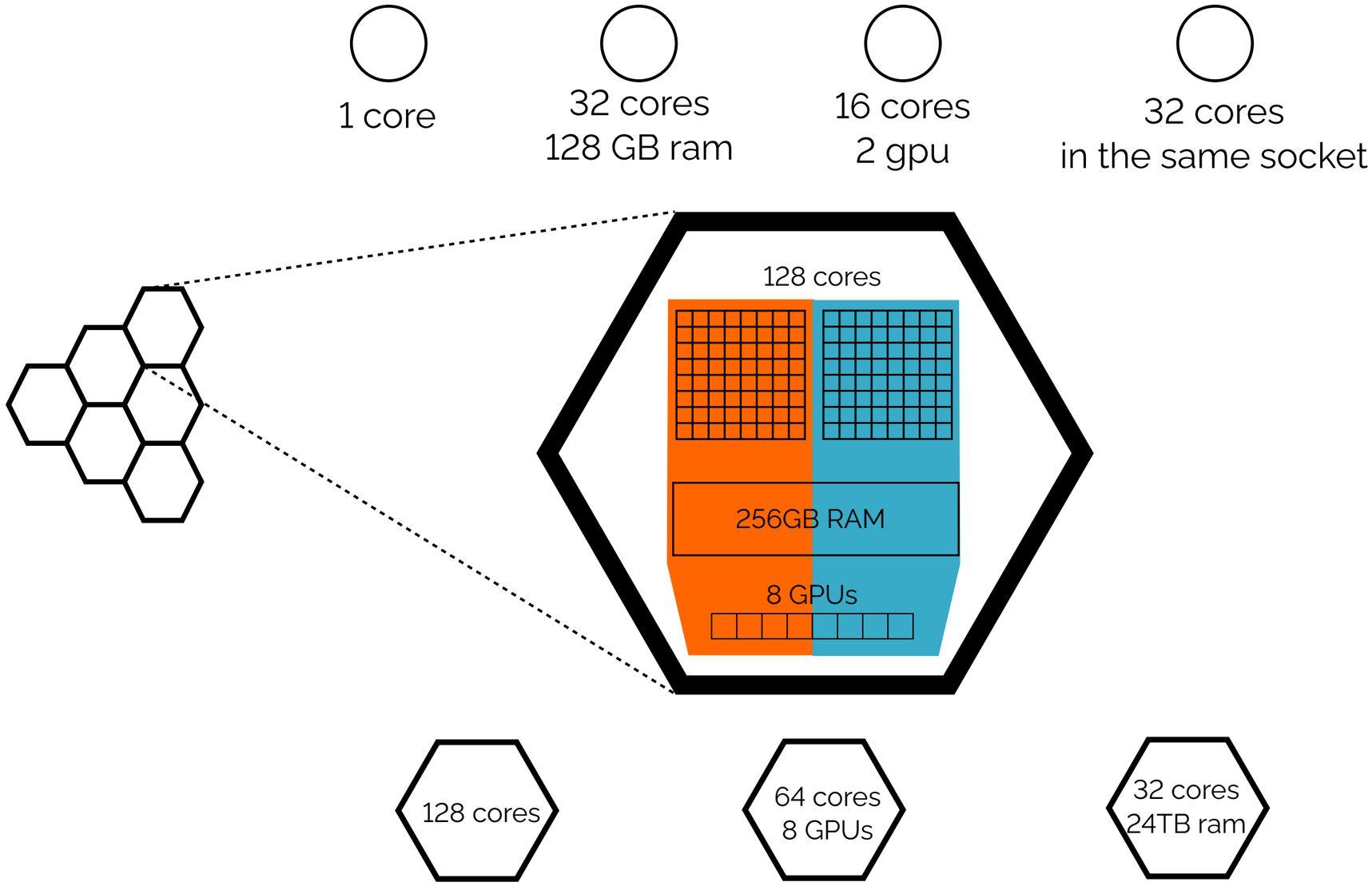

Other workflow challenges on HPC

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- Scalability

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- Fault tolerance

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- Scalability
- Multi-node tasks
- Fault tolerance
- Iterative computation

Ergonomics and **efficiency**
of workflows on HPC clusters

The Journal of Supercomputing
https://doi.org/10.1007/s11227-022-04438-y

Check for updates

Analysis of workflow schedulers in simulated distributed environments

Jakub Beránek[1] · Stanislav Böhm[1] · Vojtěch Cima[1]

Accepted: 10 March 2022

Abstract
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Keywords Distributed computing · DAG scheduling · Task Scheduling · Network models

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- Which factors affect scheduling the most?
- How can we simplify scheduler prototyping?

ESTEE

Framework for simulating workflow execution

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t0 = dag.new_task(duration=1, cpus=1, output_size=50)
t1 = dag.new_task(duration=1, cpus=1)
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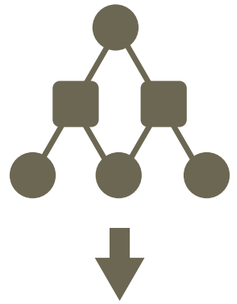
Task graph



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scheduler = BlevelGtScheduler()
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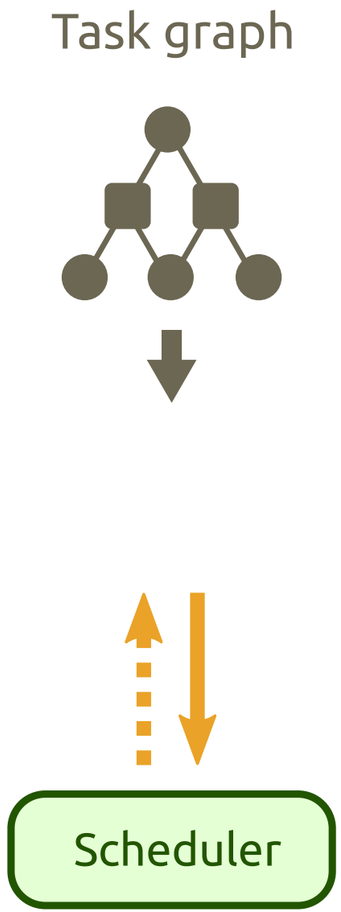

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cluster   = [Worker(cpus=8) for _ in range(3)]
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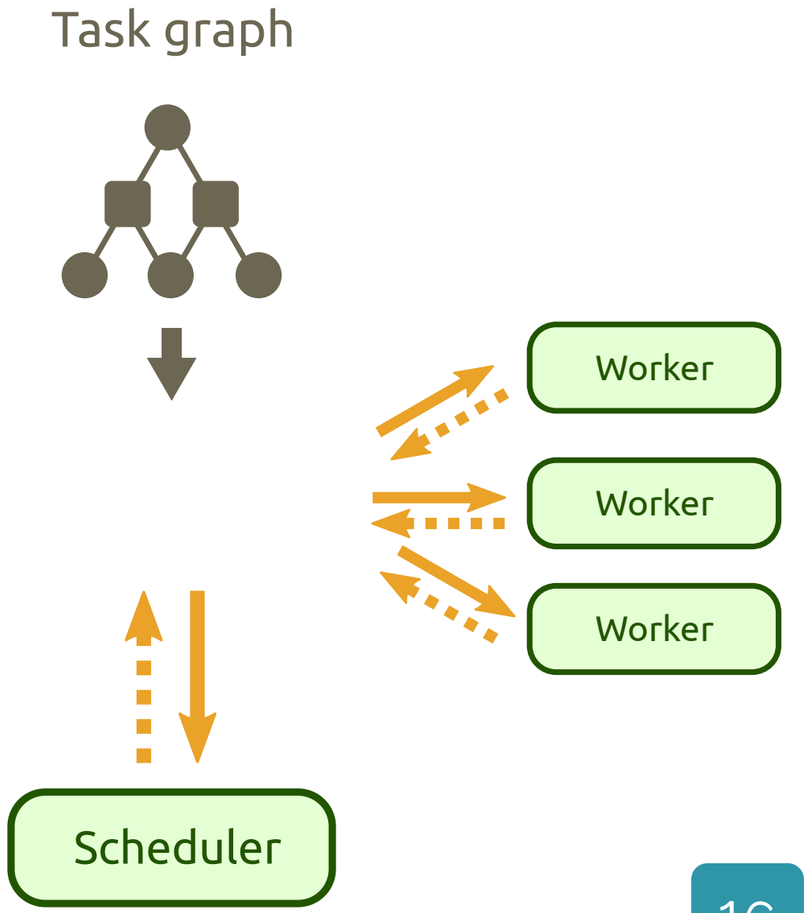

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network   = MaxMinFlowNetModel(bandwidth=10*1024)
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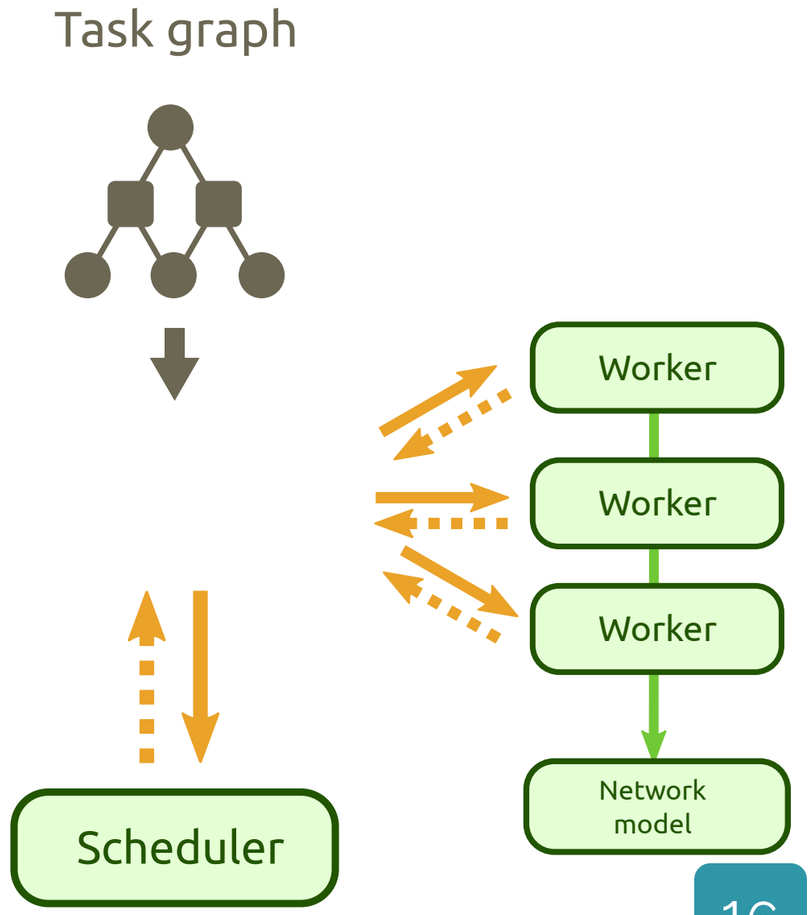

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simulator = Simulator(task_graph, cluster, scheduler, network)
makespan  = simulator.run()
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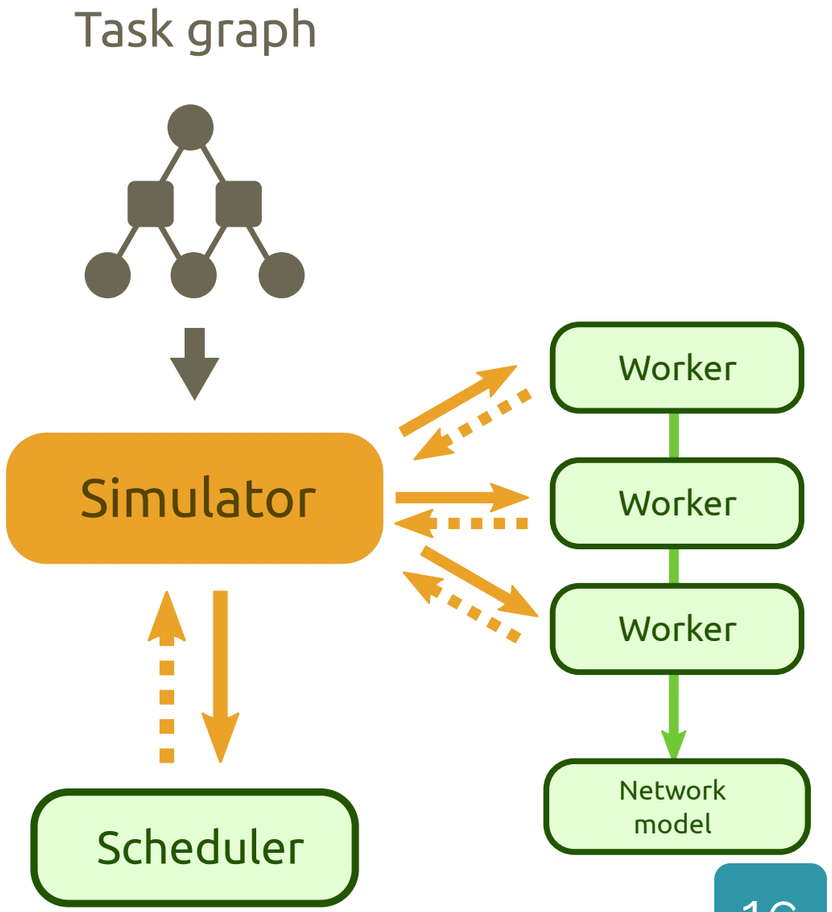

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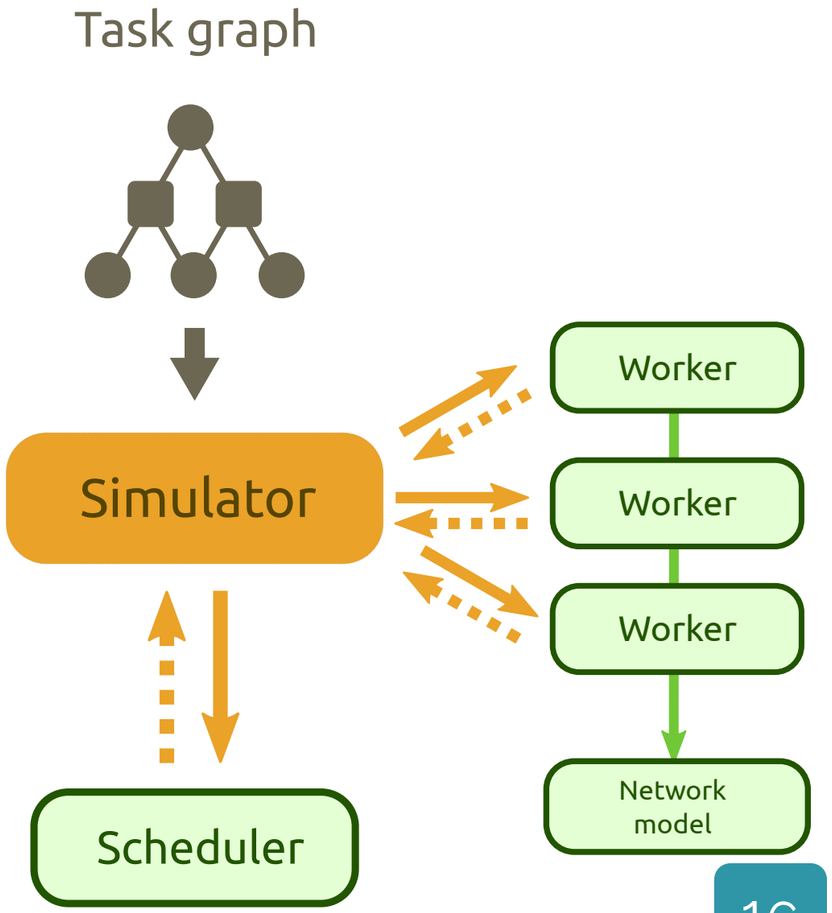

Scheduler analysis

- Compare scheduler performance

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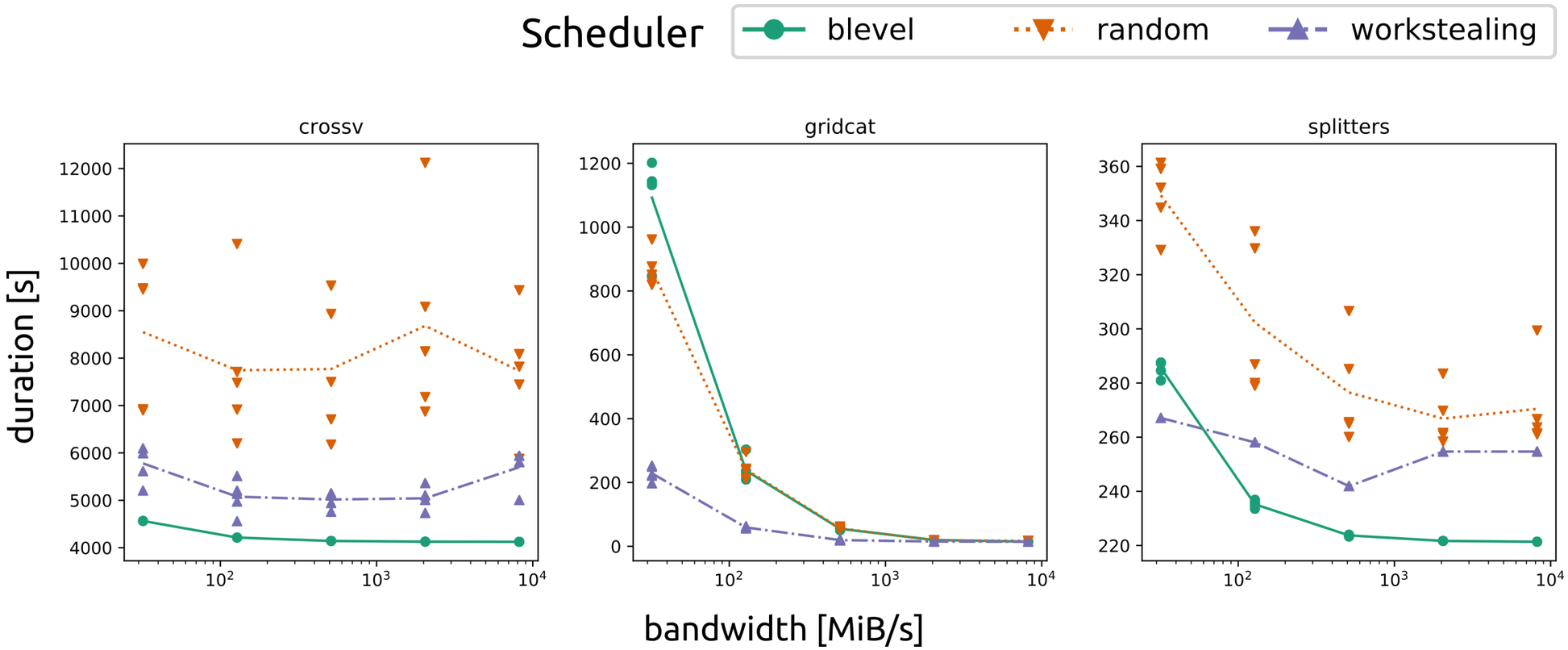
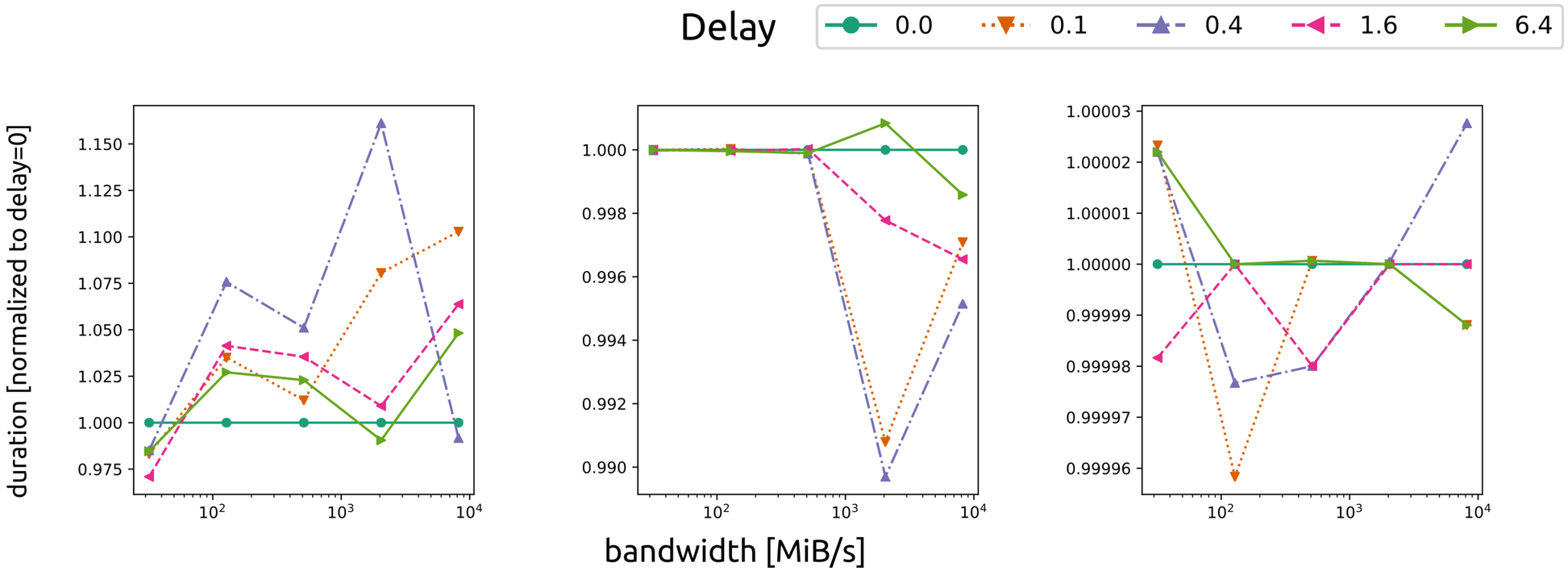
- Compare scheduler performance
- Analyze factors that affect scheduling

Runtime vs. network speed



Scheduling frequency effect



Outcome

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Outcome

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  - B-level

Outcome

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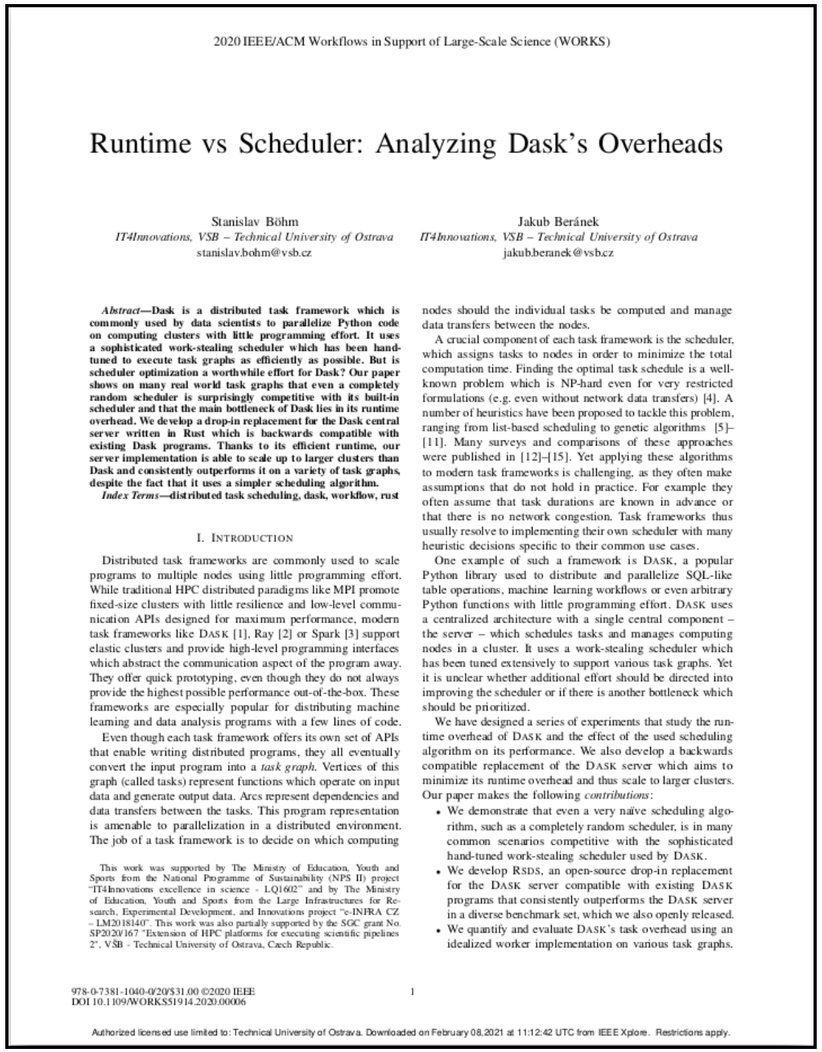

2020 IEEE/ACM Workflows in Support of Large-Scale Science (WORKS)

Runtime vs Scheduler: Analyzing Dask's Overheads

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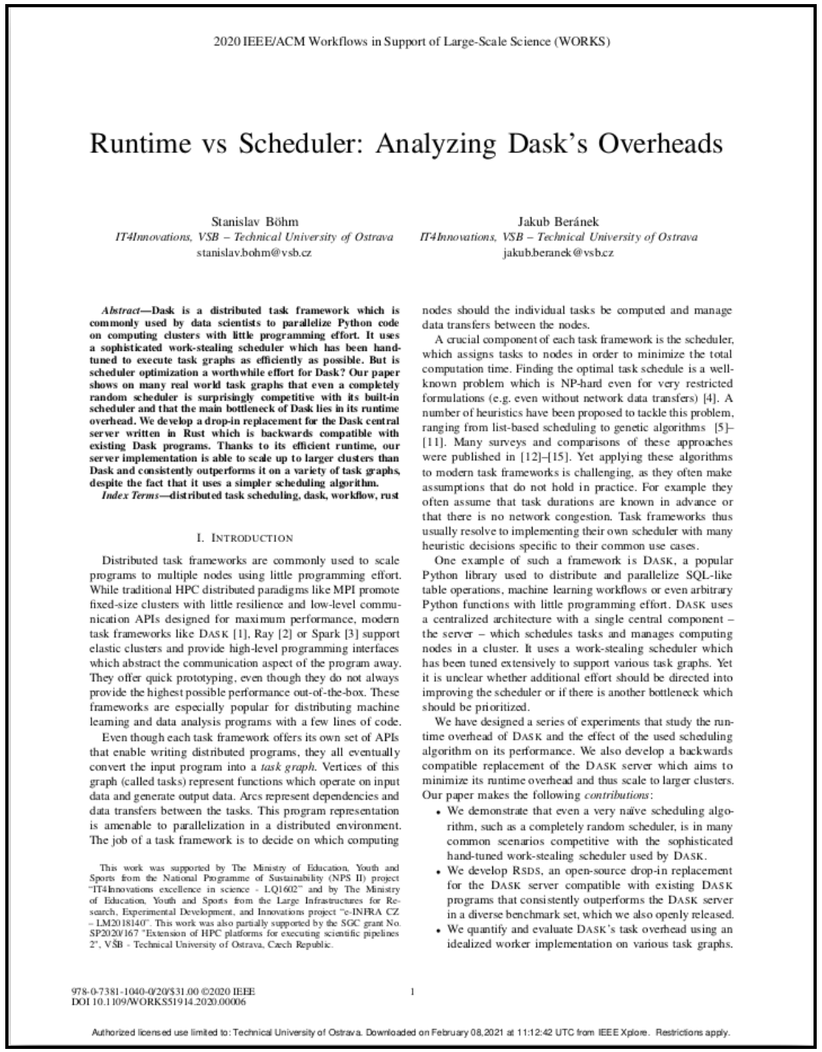

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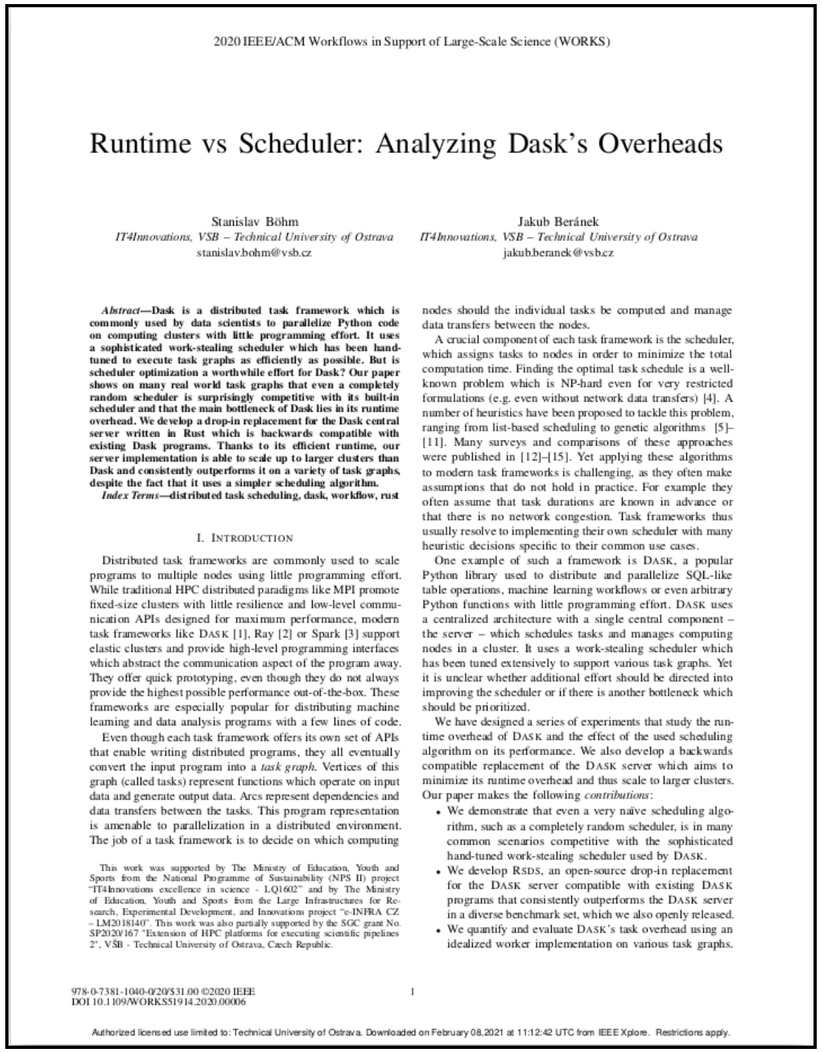

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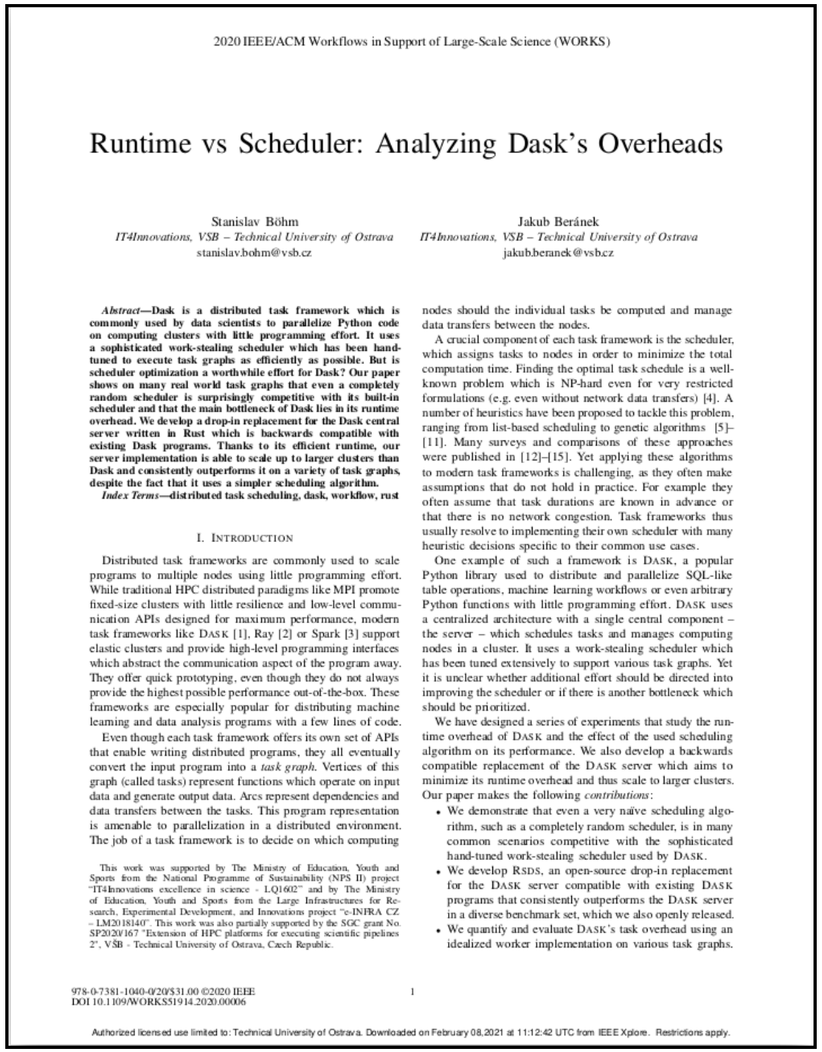

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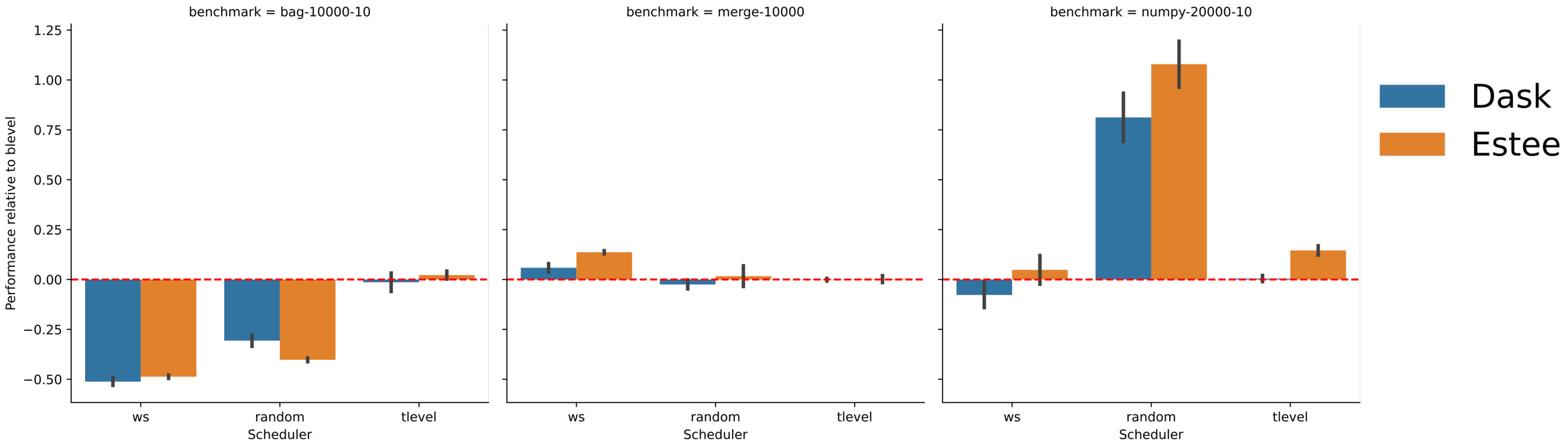
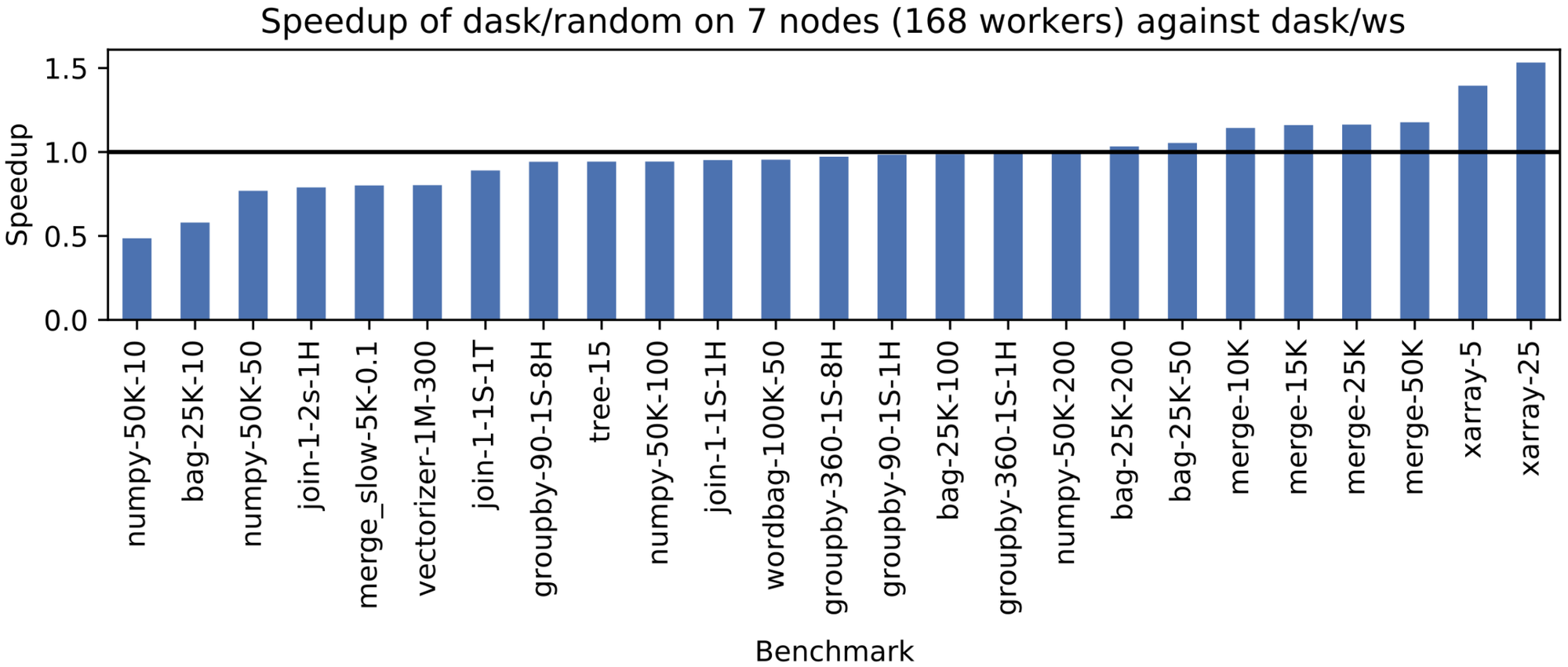
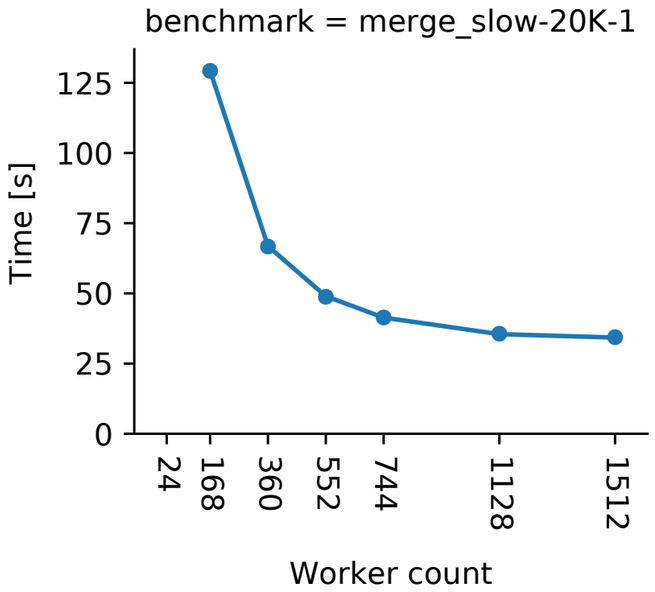
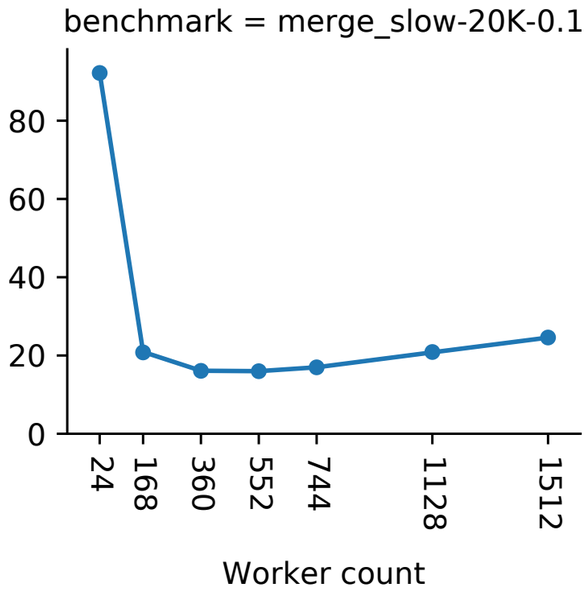


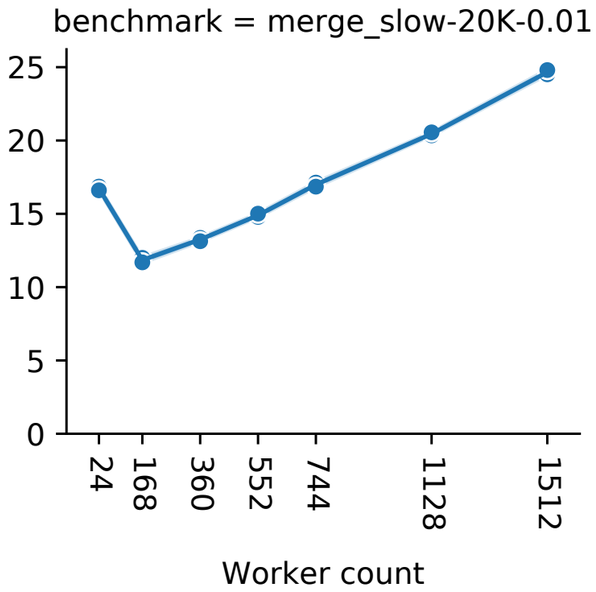
Random vs. work-stealing scheduler



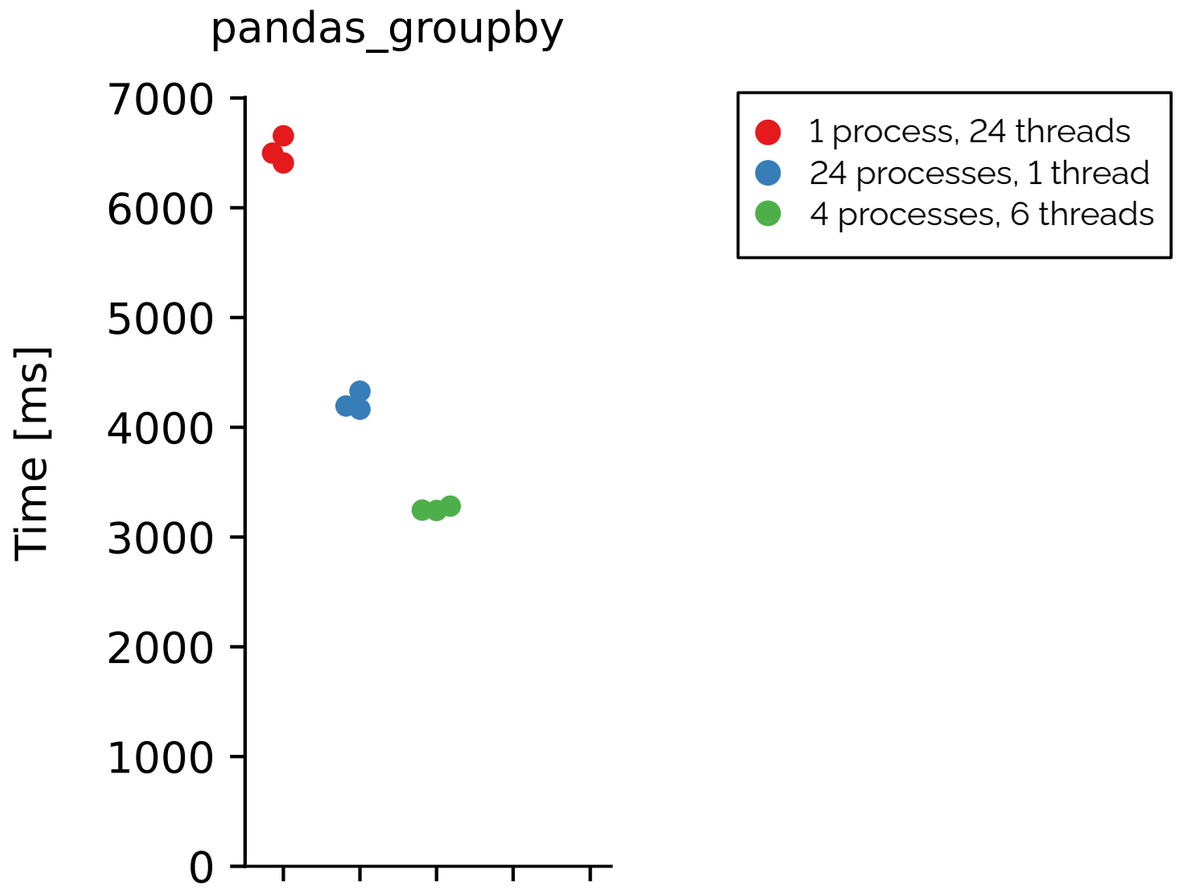
Dask scaling







Effect of GIL on Dask's performance



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RSDS

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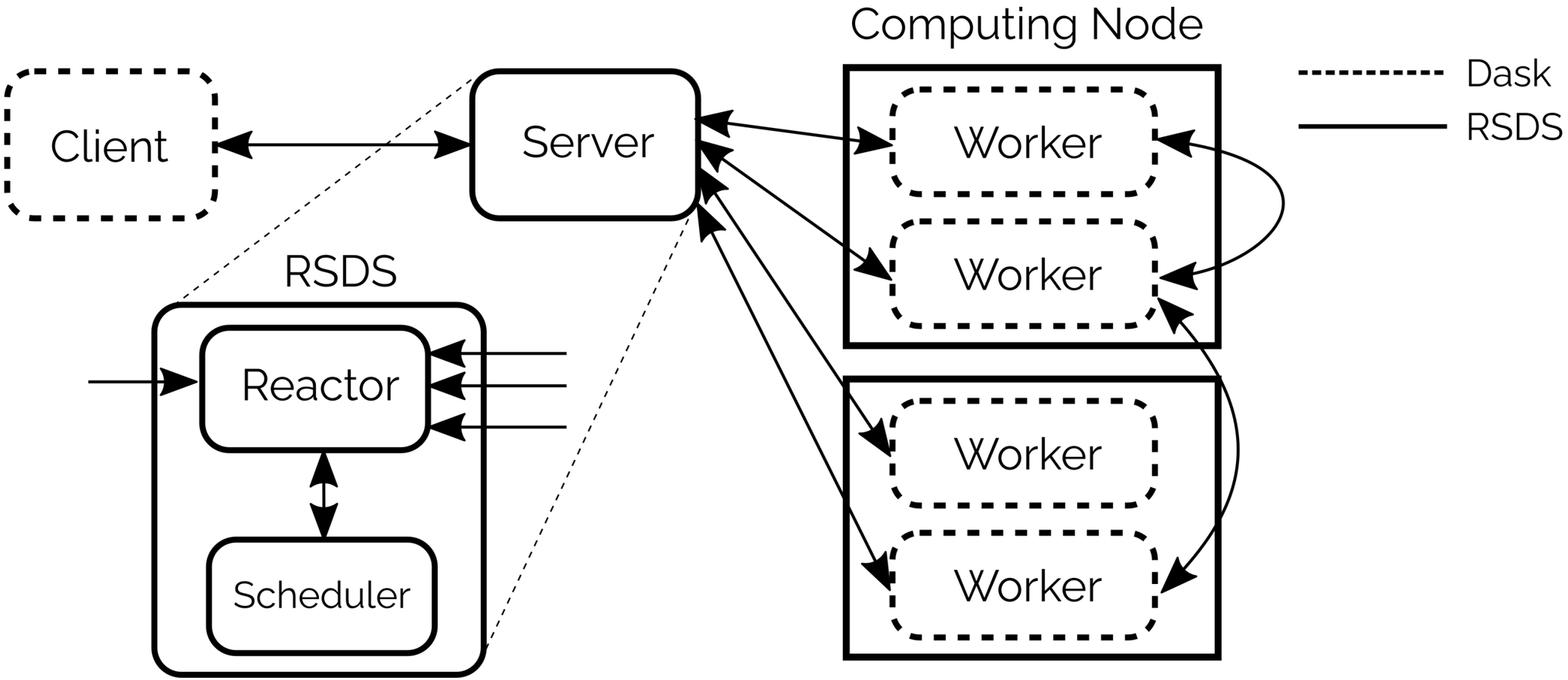
RSDS architecture



Dask vs. RSDS: work-stealing scheduler

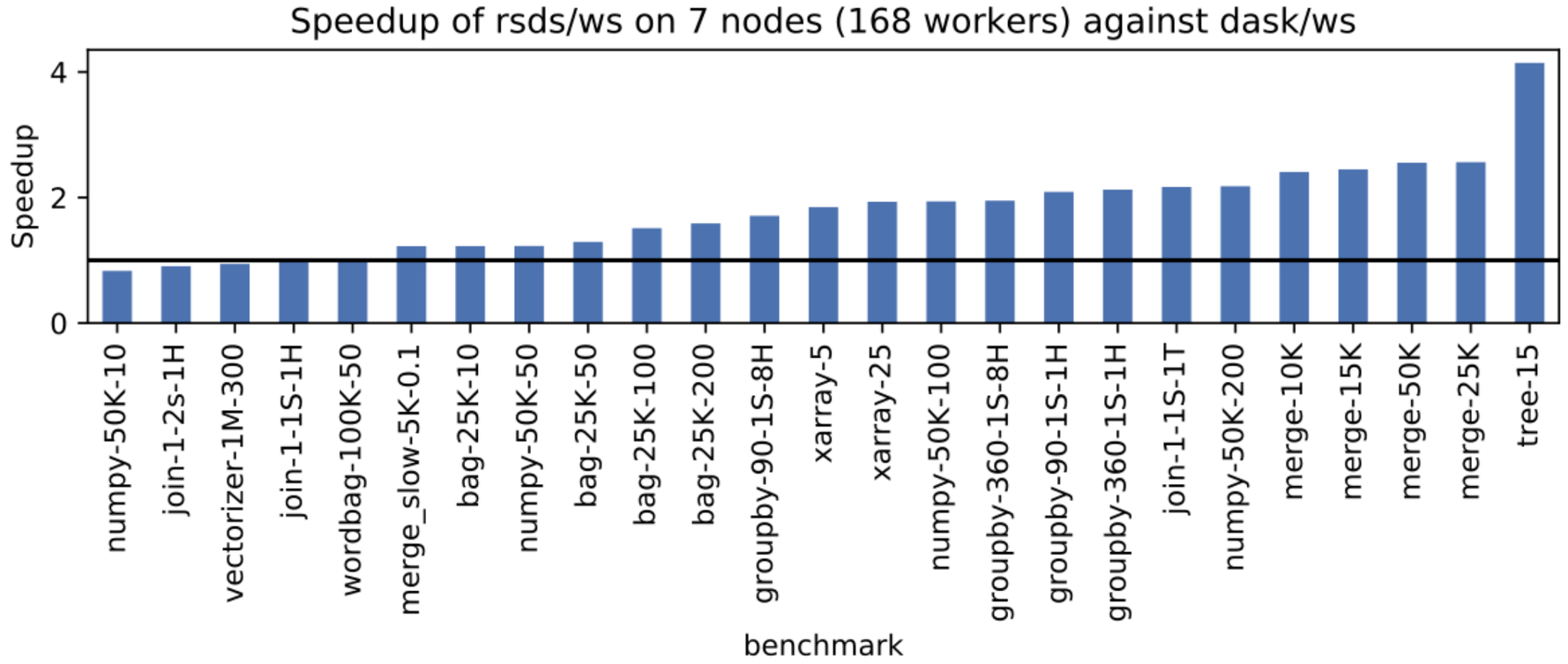
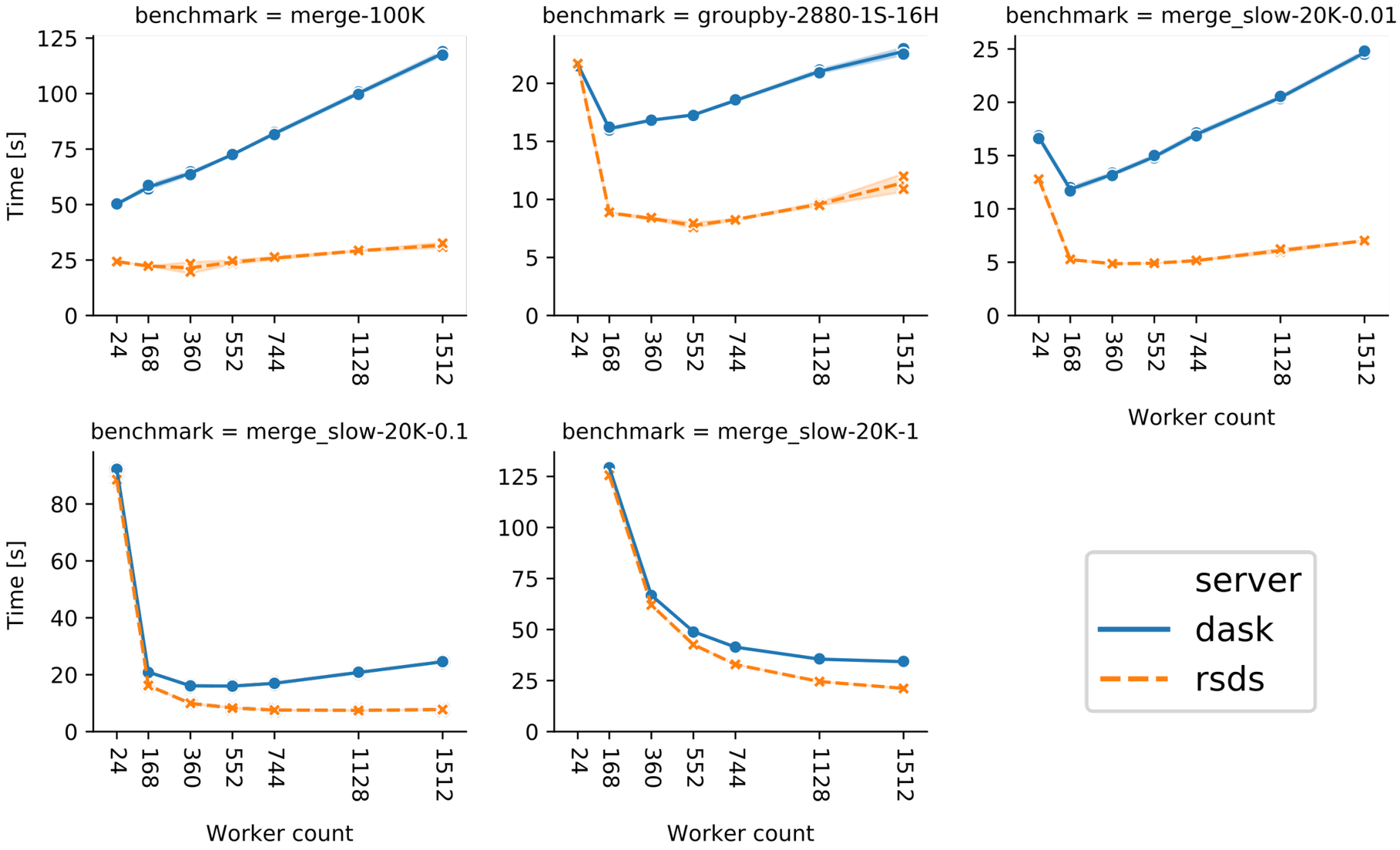


Fig. 3. Speedup of RSDS/ws scheduler; DASK/ws is baseline.

Dask vs. RSDS: scaling



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Ergonomics and efficiency
of workflows on HPC clusters

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Original software publication

HyperQueue: Efficient and ergonomic task graphs on HPC clusters

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ARTICLE INFO

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High performance computing
Job manager

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Support email for questions	jakub.beranek@vsb.cz

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  - Interaction with HPC allocation managers
  - Heterogeneous resource management
  - Scalability
- Can we integrate the solutions into a single task runtime?

Challenge: how to map tasks to allocations?

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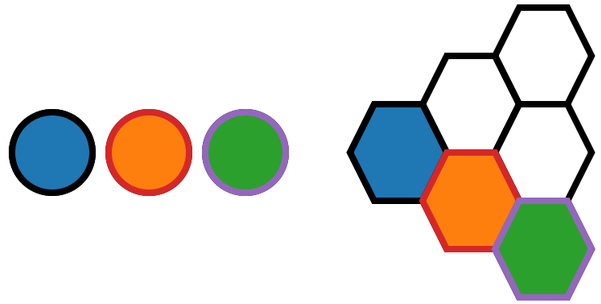
- Each task is a separate allocation
  - Massive overhead (millions of allocations)
  - Allocation count limits
  - Node granularity



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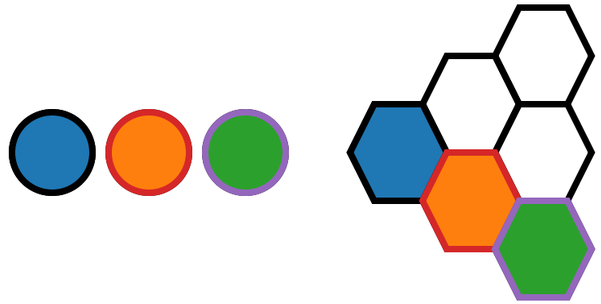
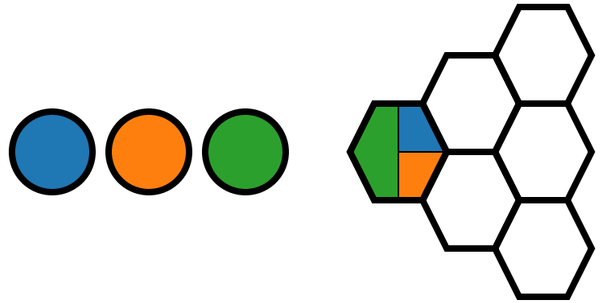


- One allocation for the whole workflow
  - Only for small workflows
  - Leads to resource waste



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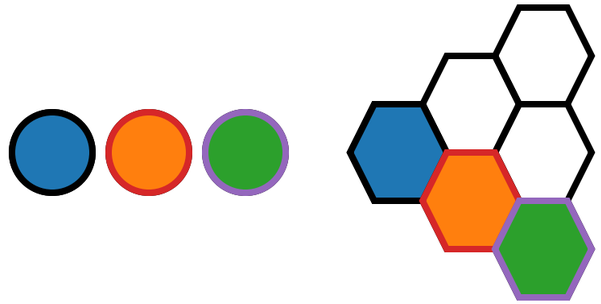

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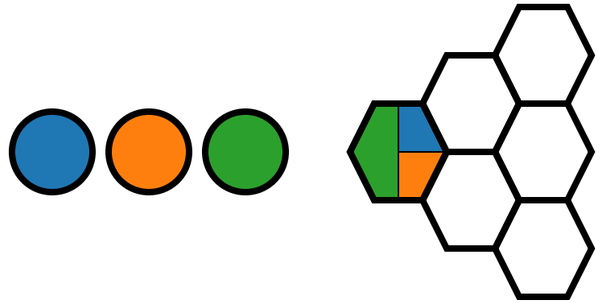
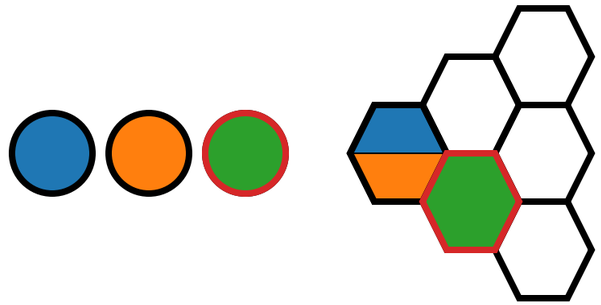


- Split workflow into multiple allocations
  - Challenging to find good partitioning
  - No load balancing across allocations
  - Dependencies and fault tolerance are problematic



Workflow partitioning

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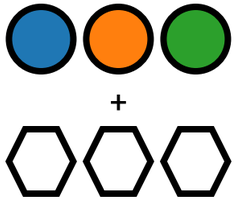
Manual (Slurm)



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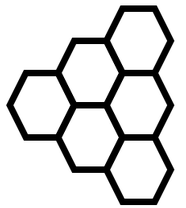

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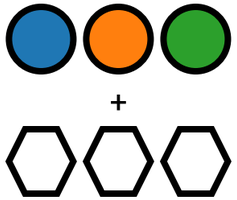

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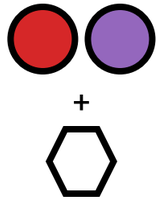

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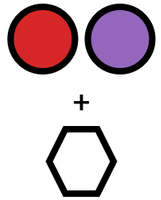

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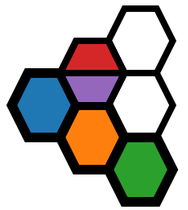
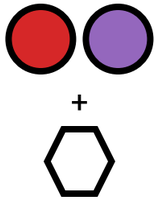


Workflow partitioning

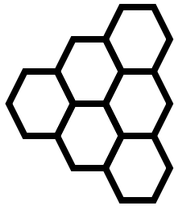
Manual (Slurm)



→ Slurm →

Meta-scheduling

→ Meta-scheduler → Slurm →



Workflow partitioning

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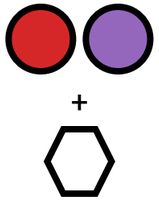

→ Slurm →

Meta-scheduling

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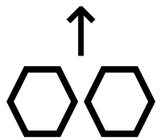

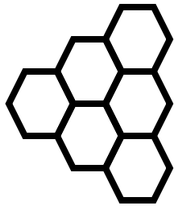

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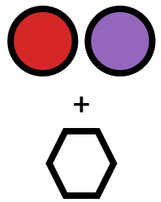
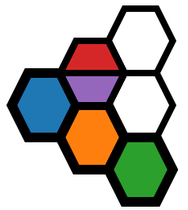


→ Slurm →



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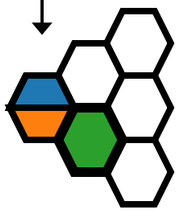
→ Meta-scheduler → Slurm →



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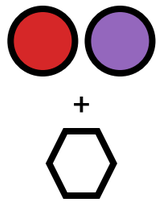

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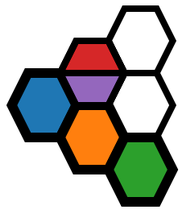
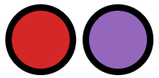
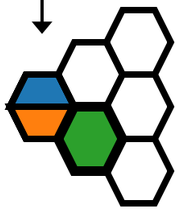
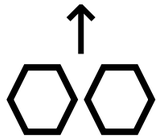


Meta-scheduling



→ Meta-scheduler → Slurm →





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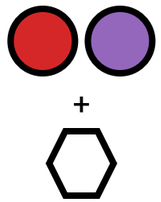

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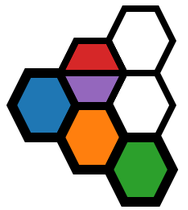

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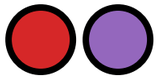

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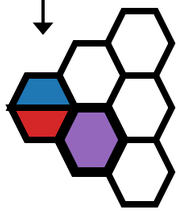

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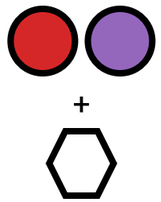

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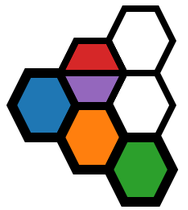

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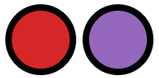

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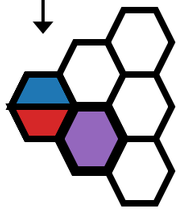
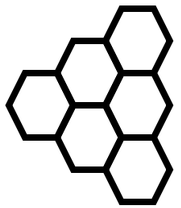


Meta-scheduling + automatic allocation

→ Meta-scheduler → Slurm →



Workflow partitioning

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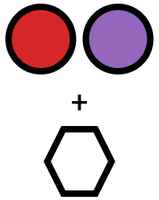

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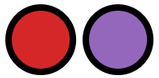

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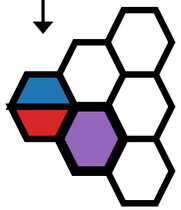

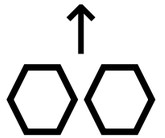

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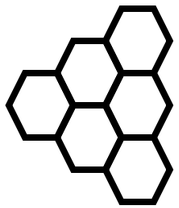

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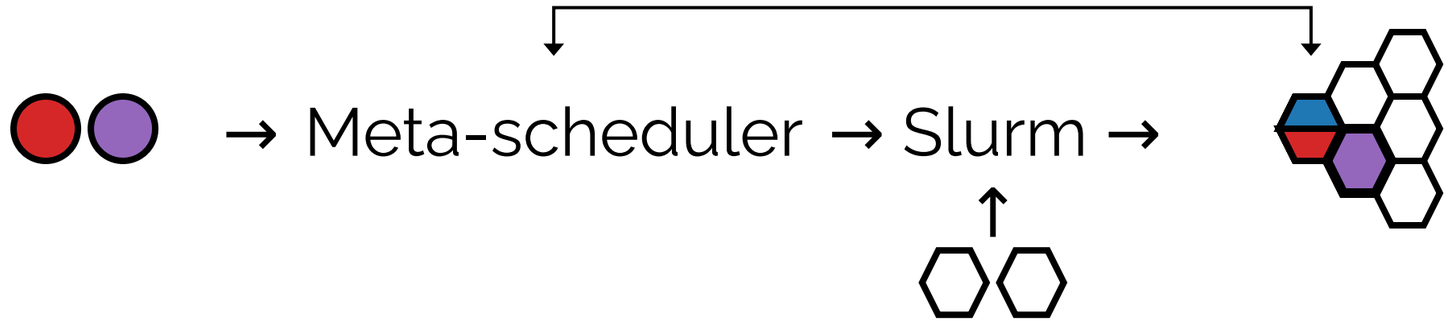

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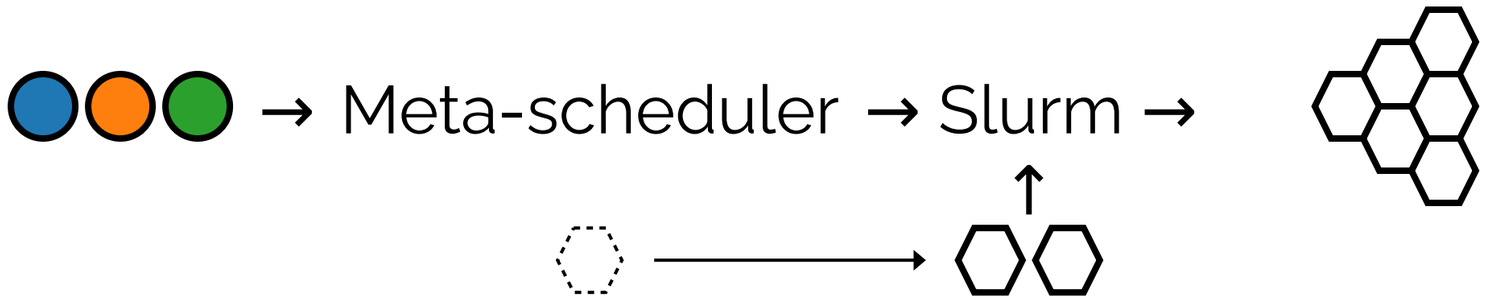

Workflow partitioning

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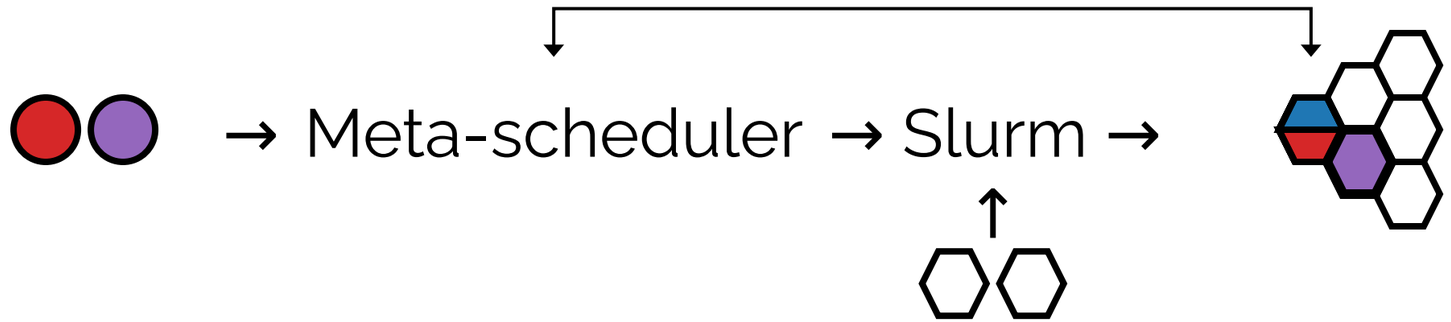

Meta-scheduling +
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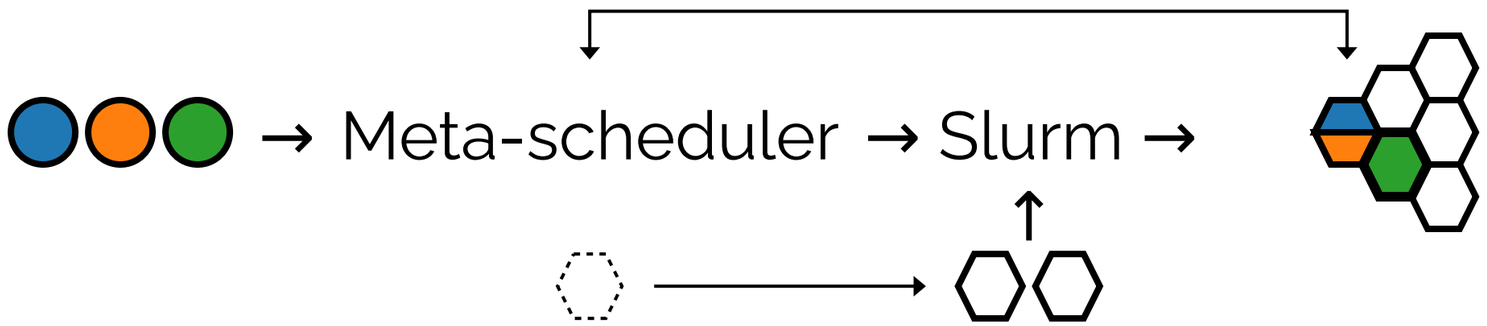

Challenge: heterogeneous resource management

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  - Task requires 0.5 of a GPU

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- Related resources
  - Task requires 4 cores in the same NUMA node
- Fractional resources
  - Task requires 0.5 of a GPU
- Resource variants
  - Task requires (1 GPU AND 1 CPU) OR 16 CPUs

HyperQueue

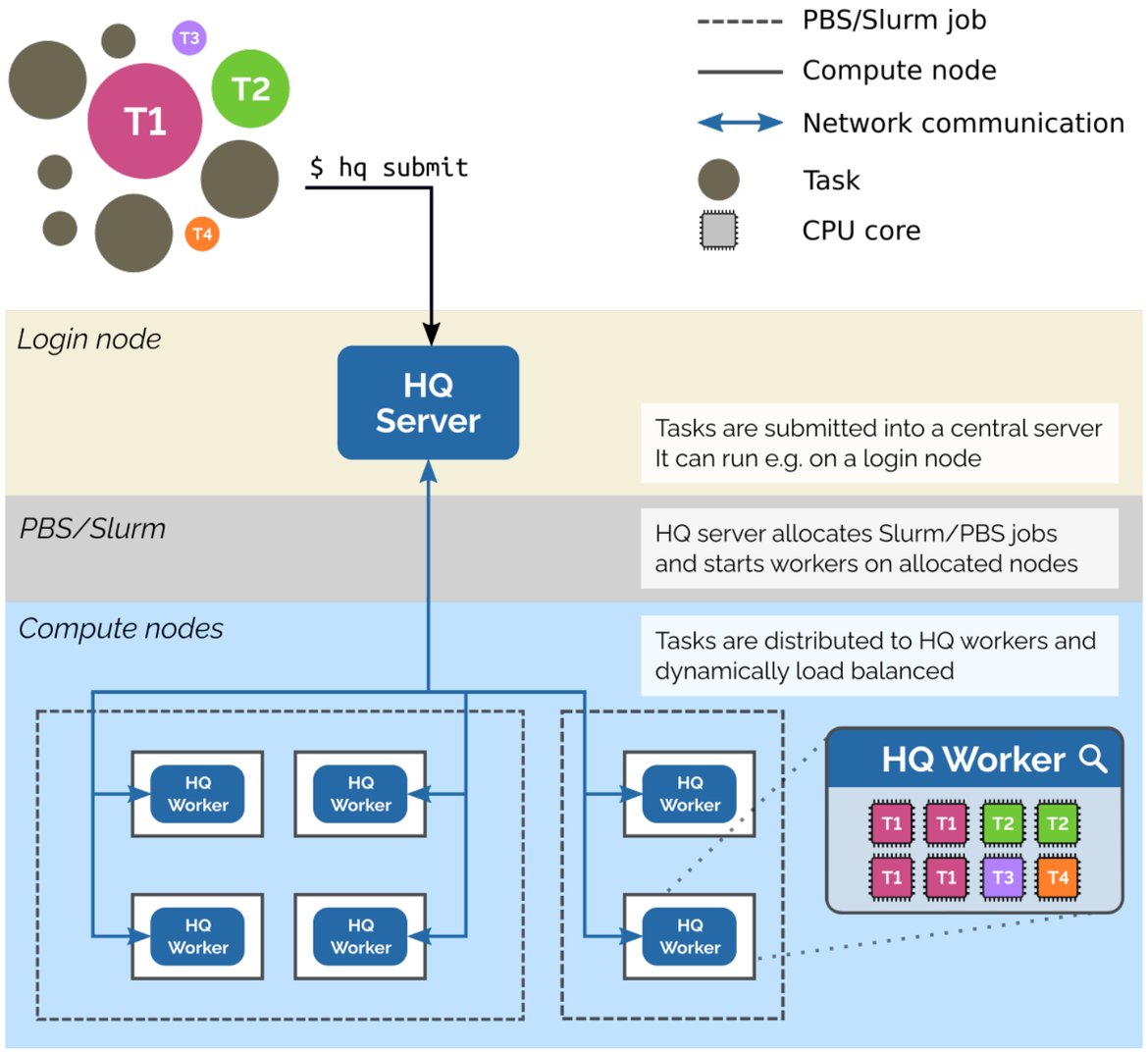
github.com/it4innovations/hyperqueue

HyperQueue

`github.com/it4innovations/hyperqueue`

Task runtime designed for HPC use-cases

Architecture



HyperQueue solutions for workflow challenges

- Meta-scheduling
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  - CLI, TOML workflow files, Python API

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- Output streaming
  - Reduces networked filesystem contention
- Several programming interfaces
  - CLI, TOML workflow files, Python API
- Trivial deployment
  - Single binary, no dependencies, no *sudo* needed

Scalability evaluation

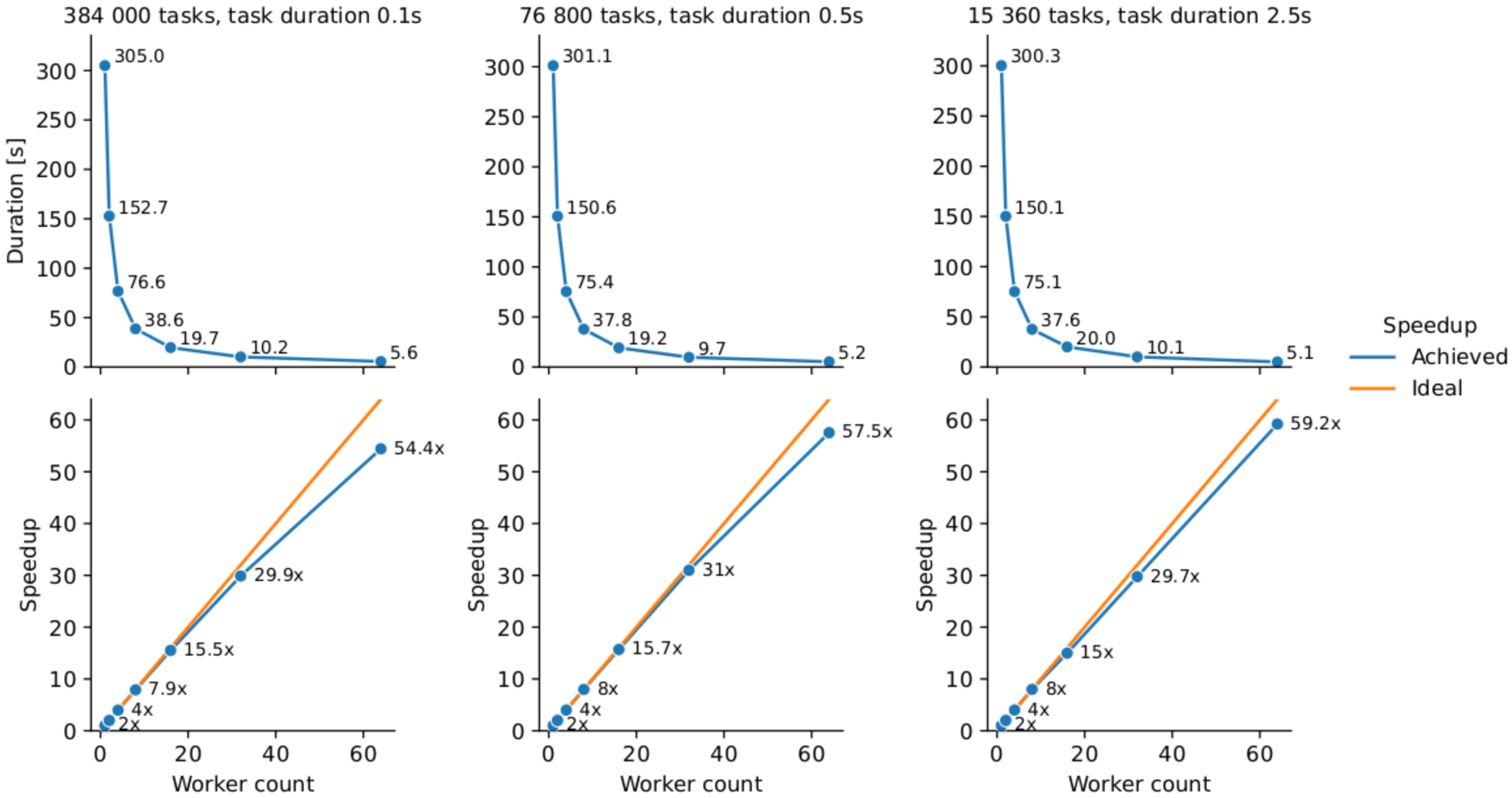

Figure 7.7: Strong scalability of HyperQueue with a fixed target makespan (300 s)

Scalability vs Dask evaluation

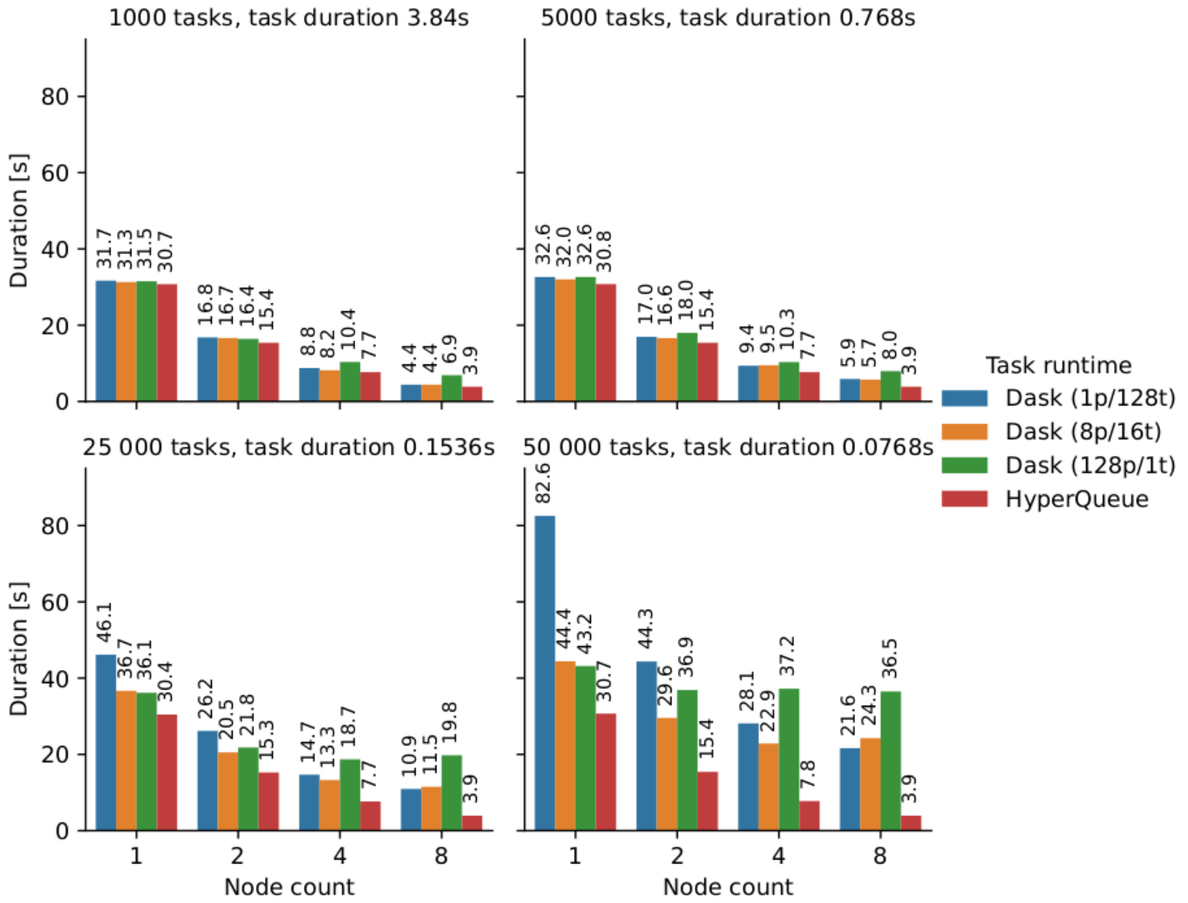

Figure 7.9: Scalability of HyperQueue vs Dask with a fixed target makespan (30 s)

Overhead evaluation

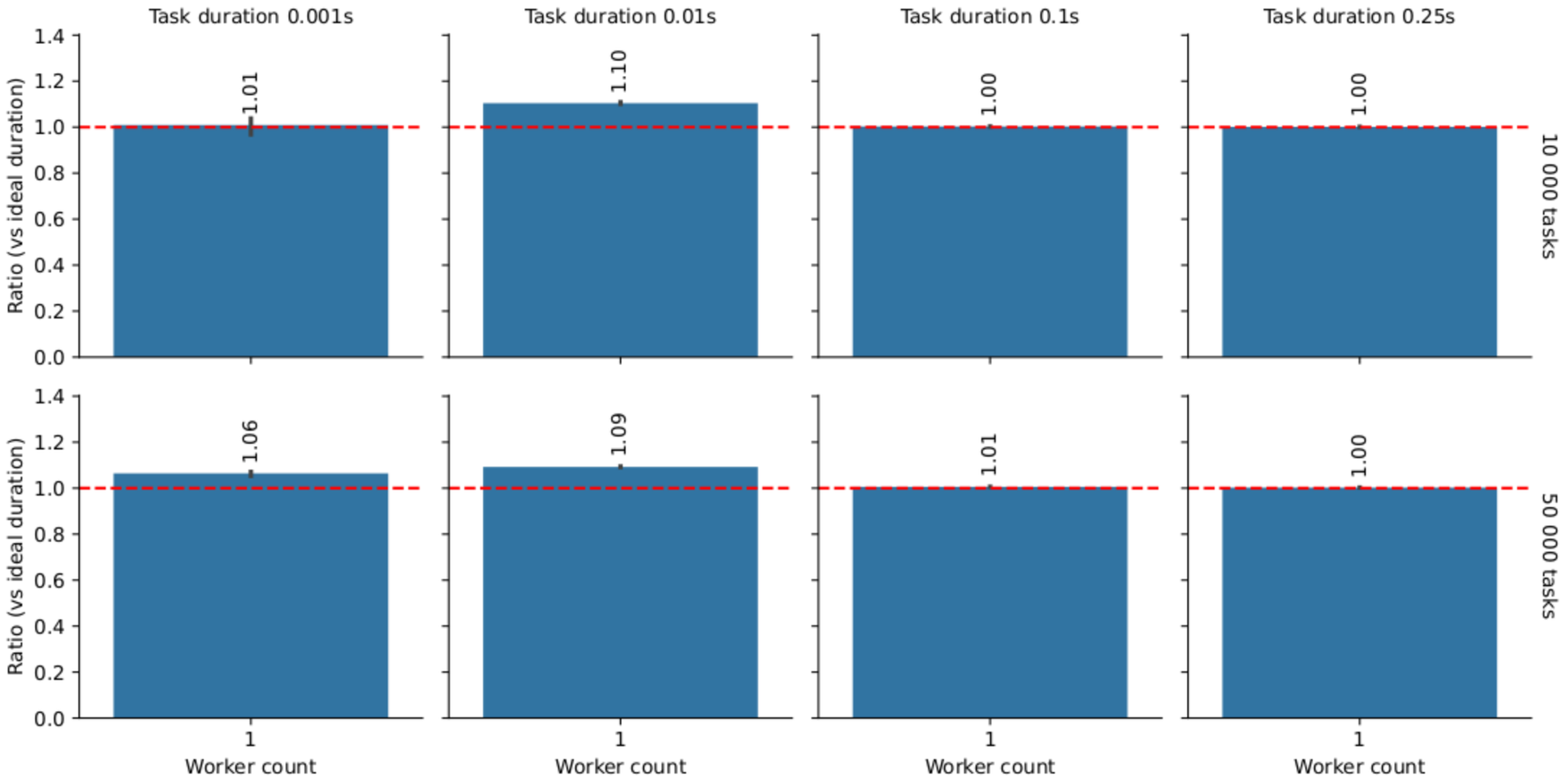

Figure 7.5: Total overhead of HyperQueue (ratio vs manual process execution)

Fractional resources evaluation

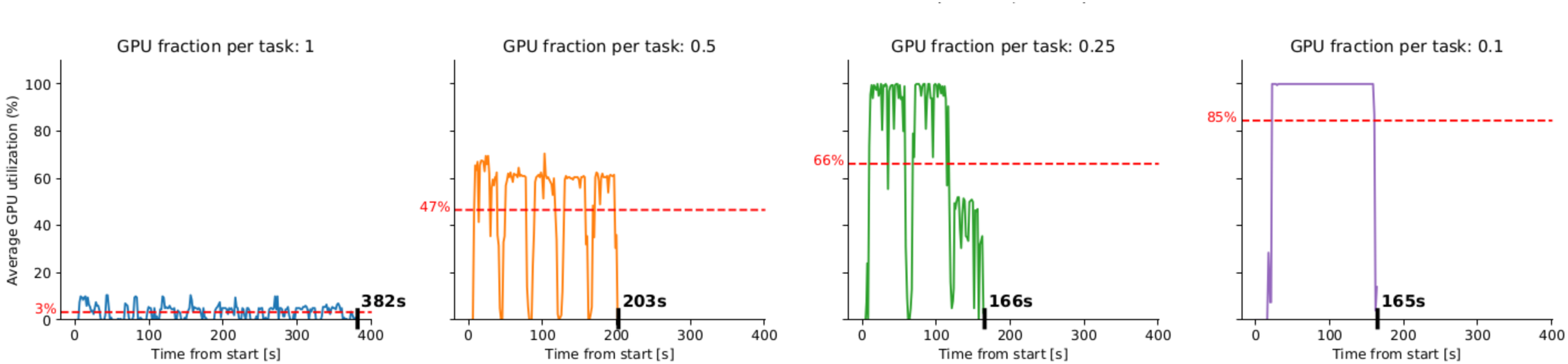

Figure 7.12: GPU hardware utilization improvements with fractional resource requirements

Comparison of HQ and similar tools

Task runtime	Task interfaces				Task dependencies		Fault tolerance		Meta-scheduling			Resources								Data transfers		Deployment
	CLI	Workflow file	Python API	Dynamic task graphs	Explicit	Inferred from files	Worker failure	Server failure	Graph partitioning	Automatic allocation	Generic workers	Basic resources	Custom resources	Non-fungible resources	Related resources	Fractional resources	Resource variants	Multi-node tasks	Directly between tasks	Output streaming	Runtime dependencies
GNU PARALLEL	👍	-	-	-	-	-	◐	-	-	-	-	-	-	-	-	-	-	-	-	👍	Perl
HYPERSHELL	👍	-	👍	-	-	-	●	👍	◐	👍	-	-	-	-	-	-	-	-	-	👍	Python
DASK	-	-	👍	👍	👍	-	●	-	●†	👍†	👍	👍	👍	-	-	-	-	-	👍	👍	Python
RAY	-	-	👍	👍	👍	-	●	👍*	●	-	👍	👍	👍	-	👍	👍	-	-	👍	👍	Python
PARSL	-	-	👍	👍	👍	-	●	-	●	👍	-	👍	-	-	-	-	-	👍	👍	-	Python
PYCOMPSS	👍	-	👍	👍	👍	-	●	👍*	◐	-	-	👍	-	-	👍	-	-	👍	👍	👍	Python, Java
PEGASUS	-	👍	👍	-	👍	👍	●	👍	◐	-	-	👍	-	-	-	-	-	-	-	👍	Python, Java, HTCondor [184]
BALSAM	-	-	👍	👍	👍	-	●	👍	●	👍	👍	👍	-	-	-	-	-	👍	👍	-	Python, PostgreSQL
AUTOSUBMIT	-	👍	-	-	👍	-	●	👍	◐	👍	-	👍	-	-	-	-	-	👍	-	-	Python
FIREWORKS	-	👍	👍	👍	👍	-	◐	👍	●	👍	👍	-	-	-	-	-	-	-	-	-	Python, MongoDB
MERLIN	-	👍	-	-	👍	-	◐	👍	●	-	-	👍	-	-	-	-	-	👍	-	-	Python, RabbitMQ/Redis
SNAKEMAKE	-	👍	👍	-	-	👍	●	-	◐	👍†	-	👍	👍	-	-	-	-	👍	-	-	Python
HYPERQUEUE	👍	👍	👍	👍	👍	-	●	👍	●	👍	👍	👍	👍	👍	👍	👍	👍	👍	-	👍	

👍 supported; - not supported; ● automatic; ◐ manual;
†with an external plugin; *with additional runtime dependencies

HyperQueue impact

- EU projects
  - 

Complex workflows, Python API
  - 

Heterogeneous resources
  - 

Multi-node tasks
  - 

Server resilience, data transfers

HyperQueue impact

- EU projects
  - LIGATE Complex workflows, Python API
  - EVEREST Heterogeneous resources
  - ACROSS Multi-node tasks
  - MAX Server resilience, data transfers
- HPC centers
  - VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER
  - LUMI
  - CINECA
  - CSC

HyperQueue impact

- EU projects
  - LIGATE Complex workflows, Python API
  - EVEREST Heterogeneous resources
  - ACROSS Multi-node tasks
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  - nextflow
  - AiiDA
  - StreamFlow
  - UM-Bridge
  - HEAppE
  - ERT

HyperQueue impact

ARC-CE+HyperQueue based submission system of ATLAS jobs for Karolina HPC

M. Svatoš, J. Chudoba, P. Vokáč

6th Users Conference of IT4Innovations

3.-4.11.2022

Introduction

For several years, the distributed computing of the ATLAS experiment at the LHC (ADC) has been granted opportunistic use of computing resources of the Czech national HPC centre, IT4Innovations. Within the ADC, resources of IT4Innovations are attached to the Czech Tier2. Implementation of HyperQueue (a tool designed to simplify execution of large workflows on HPC clusters, developed by IT4Innovations) into the previously used ARC-CE based submission system allows tweaking of submitted jobs and hopefully helps with handling of pre-emption at IT4Innovations.

Submission system

Harvester, ARC-CE, sshfs, login node, HyperQueue server, ssh, Panda Server, http proxy (squid), http, PBS Pro, Storage, webdav /xroot, Lustre, Czech Tier2, IT4I

- the ARC-CE receives a pilot job, translates the job description into a script that can be run in the batch system, puts necessary files into a folder shared with the HPC via sshfs, and submits the job via ssh connection to the HyperQueue server running on a login node
- the HyperQueue server buffers the jobs and when there are enough of them, it submits jobs into the PBS Pro
- when the PBS job starts, HyperQueue jobs start in it (in sufficient numbers to fill the worker node - if available)
- in each HyperQueue job, pilot starts
- pilot contacts panda server through http proxy (Czech Tier2 squid) to receive payload job (as http is one of few open ports)
- when it receives a payload job, it gets input file from the Czech Tier2 storage via xroot or webdav (in a rucio container)
- then it starts the calculation (in software container)
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2021:Migration to HyperQueue

Testing:Efficiency (CPU/Wall) | Testing:Number of cores | Production:Number of cores | Production:Walltlock | Production:Efficiency(CPU/Wall)

- In December 2021, the HyperQueue implementation was tested on Karolina using 16 and 32 cores and then put into production a few days before the year-end

2022: Living with pre-emption

Number of cores used on Karolina and Barbora | Efficiency (CPU/Wall) on Karolina and Barbora | Number of successful and failed jobs on Karolina and Barbora | Number of cores used by all Czech Tier2 resources | CPU consumption of all Czech Tier2 resources

- In 2022, new project which can use only pre-emptive queues started in September.
- Development to tune the submission system continues.
- Contribution of Barbora, which is not using the HyperQueue yet, is not significant in comparison with Karolina.
- Even with pre-emption, the IT4I provides significant resources to Czech Tier2 with high efficiency.

Acknowledgement

This work and computing resources at FZU were co-financed by projects CERN-C (CZ.02.1.01/0.0/0.0/16013/0001404) and CERN-CD (CZ.02.1.01/0.0/0.0/18_046/0016013) from EU funds and MSMT and projects CERN-CZ (LM2018104) and LTT17018.

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2021:Migration to HyperQueue

Testing:Efficiency (CPU/Wall), Testing:Number of cores, Production:Number of cores, Production:Walltclock, Production:Efficiency(CPU/Wall)

32 cores, 16 cores, 128 cores, 90%

- In December 2021, the HyperQueue implementation was tested on Karolina using 16 and 32 cores and then put into production a few days before the year-end

2022: Living with pre-emption

Number of cores used on Karolina and Barbora, Efficiency (CPU/Wall) on Karolina and Barbora, Number of successful and failed jobs on Karolina and Barbora, Number of cores used by all Czech Tier2 resources, CPU consumption of all Czech Tier2 resources

Karolina, Barbora, GRID, HPC, BOINC, HPC(43%), GRID(56%)

- In 2022, new project which can use only pre-emptive queues started in September.
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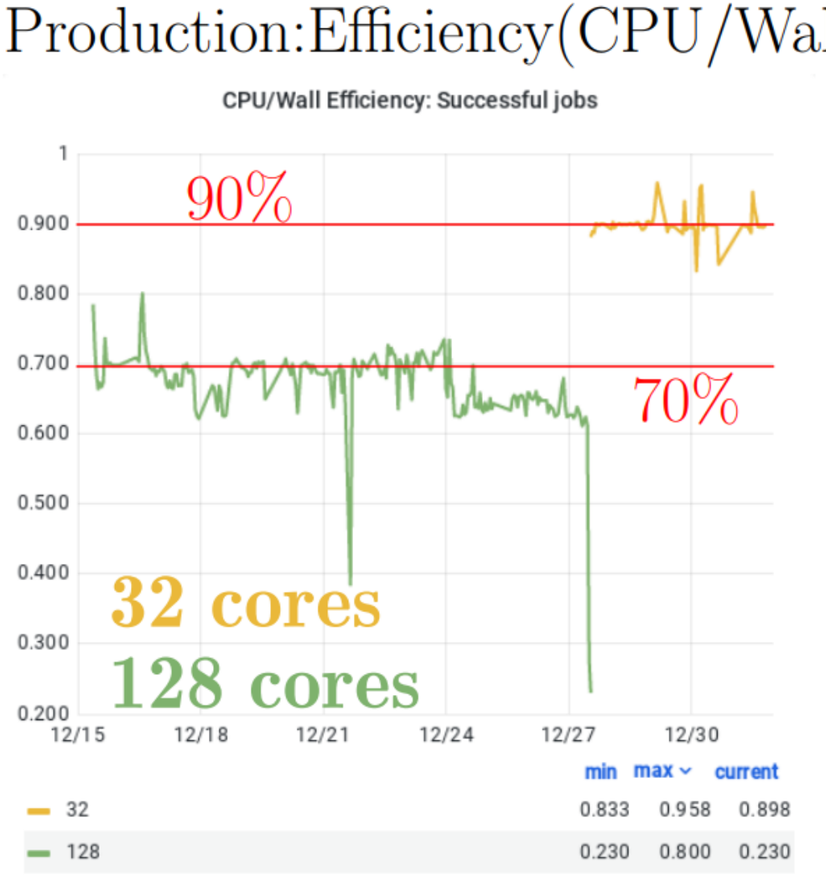

HyperQueue impact

LIGATE Pose selector workflow

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- 6M+ MD simulations on 4k+ ligands
- 240k GPU hours on LUMI-G cluster
- 2M CPU hours on MeluXina cluster

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> “
> ...making both workflows some of the largest molecular dynamics campaigns ever performed...
> LIGATE Deliverable D7.1 (lessons learned) ”

Outcome

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- Integrated solution for workflows on HPC

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- Ergonomics
  - Meta-scheduling
  - Fine-grained heterogeneous resource management
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- Open source
  -  `github.com/it4innovations/hyperqueue`

Thesis objectives fulfillment

1. Identify HPC workflow challenges ✓

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   - HyperQueue
4. Analyze results on real use-cases ✓
   - LIGATE, CERN

Thank you for your attention

Slides made with https://github.com/spirali/elsie

Publications related to thesis

- **Analysis of workflow schedulers in simulated distributed environments**
  Jakub Beránek, Ada Böhm, Vojtěch Cima
  The Journal of Supercomputing 2022

- **Runtime vs Scheduler: Analyzing Dask's Overheads**
  Ada Böhm, *Jakub Beránek*
  IEEE/ACM Workflows in Support of Large-Scale Science (WORKS) 2020

- **HyperQueue: Efficient and ergonomic task graphs on HPC clusters**
  Jakub Beránek, Ada Böhm, Gianluca Palermo, Jan Martinovič, Branislav Jansík
  SoftwareX 2024

Publications unrelated to thesis

Network-Accelerated Non-Contiguous Memory Transfer
S. Di Girolamo, K. Taranov, A. Kurth, M. Schaffner, T. Schneider, *J. Beránek*, M. Besta, L. Benini, D. Roweth, T. Hoefler
SC (International Conference for High Performance Computing, Networking, Storage and Analysis) 2019

Streaming Message Interface: High-Performance Distributed Memory Programming on Reconfigurable Hardware
T. De Matteis, J. de Fine Licht, *J. Beránek*, T. Hoefler
SC (International Conference for High Performance Computing, Networking, Storage and Analysis) 2019

A RISC-V in-Network Accelerator for Flexible High-Performance Low-Power Packet Processing
S. Di Girolamo, A. Kurth, A. Calotoiu, T. Benz, T. Schneider, *J. Beránek*, L. Benini, T. Hoefler
ISCA (International Symposium on Computer architecture) 2021

SISA: Set-Centric Instruction Set Architecture for Graph Mining on Processing-in-Memory System
M. Besta, R. Kanakagiri, G. Kwasniewski, R. Ausavarungnirun, *J. Beránek*, K. Kanellopoulos, K. Janda, Z. Vonarburg-Shmaria, L. Gianinazzi, I. Stefan, J. G. Luna, J. Golinowski, M. Copik, L. Kapp-Schwoerer, S. Di Girolamo, N. Blach, M. Konieczny, O. Mutlu, T. Hoefler
IEEE/ACM MICRO (International Symposium on Microarchitecture) 2021

GraphMineSuite: Enabling High-Performance and Programmable Graph Mining Algorithms with Set Algebra
M. Besta, Z. Vonarburg-Shmaria, Y. Schaffner, L. Schwarz, G. Kwasniewski, L. Gianinazzi, *J. Beránek*, K. Janda, T. Holenstein, S. Leisinger, P. Tatkowski, E. Ozdemir, A. Balla, M. Copik, P. Lindenberger, M. Konieczny, O. Mutlu, T. Hoefler
PVLDB 2021

Tunable and Portable Extreme-Scale Drug Discovery Platform at Exascale: The LIGATE Approach
G. Palermo, G. Accordi, D. Gadioli, E. Vitali, C. Silvano, B. Guindani, D. Ardagna, A. Beccari, D. Bonanni, C. Talarico, F. Lughini, J. Martinovič, P. Silva, A. Böhm, *J. Beránek*, J. Křenek, B. Jansík, B. Cosenza, L. Crisci, P. Thoman, P. Salzmann, T. Fahringer, L. Alexander, G. Tauriello, T. Schwede, J. Durairaj, A. Emerson, F. Ficarelli, S. Wingbermühle, E. Lindahl, D. Gregori, E. Sana, S. Coletti, P. Gschwandtner
Proceedings of the 20th ACM International Conference on Computing Frontiers

pyCaverDock: Python implementation of the popular tool for analysis of ligand transport with advanced caching and batch calculation support
O. Vávra, *J. Beránek*, J. Šťourač, M. Šurkovský, J. Filipovič, J. Damborský, J. Martinovič, D. Bednář
Bioinformatics 2023

Haydi: Rapid Prototyping and Combinatorial Objects
Stanislav Böhm, *Jakub Beránek*, Martin Šurkovský
Foundations of Information and Knowledge Systems 2018

Alternative Paths Reordering Using Probabilistic Time-Dependent Routing
M. Golasowski, *J. Beránek*, M. Šurkovský, L. Rapant, D. Szturcová, J. Martinovič, Kateřina Slaninová
Advances in Networked-based Information Systems 2020

A Distributed Environment for Traffic Navigation Systems
J. Martinovič, M. Golasowski, K. Slaninová, *J. Beránek*, M. Šurkovský, L. Rapant, D. Szturcová, R. Cmar
Complex, Intelligent, and Software Intensive Systems 2020

Question 1 (doc. Mgr. Jiří Dvorský, Ph.D.)

> “
> Will it be possible to apply HyperQueue to a quantum computer as well?
> ”

Question 1 (prof. Ismail Hakki Toroslu)

> “
> The thesis identifies key challenges in task scheduling and resource management on heterogeneous supercomputers. What are the most significant bottlenecks and how RSDS or HyperQueue addresses these bottlenecks?
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- HQ: meta-scheduling, heterogeneous resource management

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- Specialized use-cases
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- Latency (not throughput) optimized scheduling

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> Thesis mentions that Python runtime overhead is a critical bottleneck in Dask. How Rust-based server (RSDS) reduces this overhead, and why Rust was chosen for this task over other languages?
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- Memory safety, data race safety

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- Missing features (data transfers, extended Python API)
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> Does the support of only acyclic task graphs may impose less efficient solutions in cases where loops involved regions of tasks? What kind of advantages and disadvantages do you see in using acyclic task graphs? Do the iterative task graphs transformed into acyclic task graphs (such as L-DAG), or each iteration as a separate task, fully solve the problem without disadvantages?
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- Dynamic loop count => dynamic tasks

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- Task runtimes should adopt to the granularity required by its users

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- Potential future work for HyperQueue

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- Experimental research: represent task graphs with finite automata

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- Dependency/resource information is embedded in the DAG
- Configuration depends on the interface (Python, CLI, TOML)
- HQ uses structural sharing for shared requirements

Question 6 (assoc. prof. João Manuel Paiva Cardoso)

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- Tasks are resilient to worker failures (task instances)
- Tasks are resilient to server failures (journaling)
- Potential future work: task checkpointing

Question 7 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The example in Fig. 3.2 seems to not consider the different execution time of tasks according to the worker. When there are differences, for instance because of the use of different computing units (CPU vs GPU), how does the scheduling decide? What kind of possibilities do you see if we also consider variants of the tasks, using the same CPU, but with different energy/execution time trade-offs?
> ”

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according to t
use of differer
What kind of p
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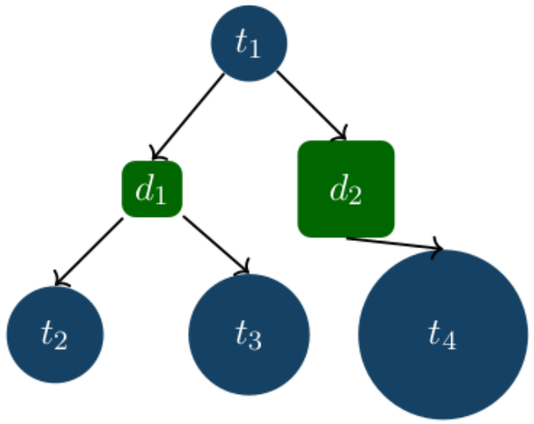

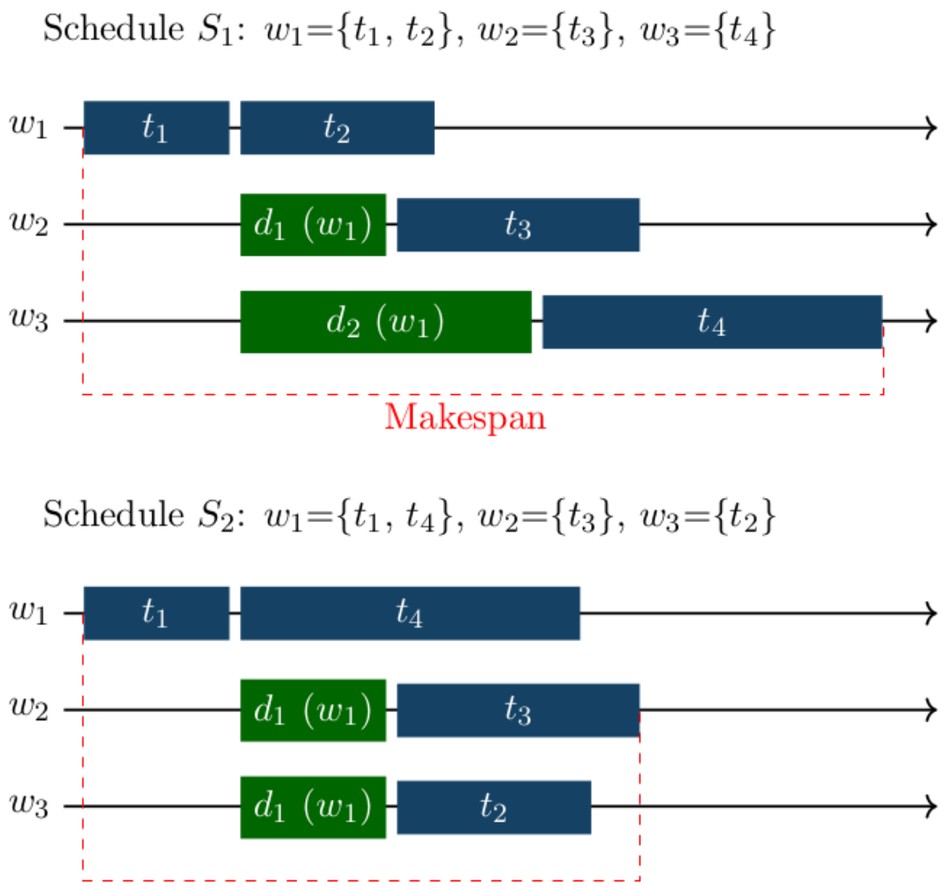

Figure 3.2: Task graph executed with two different schedules

Question 8 (assoc. prof. João Manuel Paiva Cardoso)

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> The use of checkpointing, although convenient, usually introduces a large overhead. Is this overhead automatically managed or it needs to be explicitly managed by the user?
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- HQ doesn't perform task checkpointing

Question 8 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The use of checkpointing, although convenient, usually introduces a large overhead. Is this overhead automatically managed or it needs to be explicitly managed by the user?
> ”

- HQ doesn't perform task checkpointing
- HQ optionally stores a (GZIP-compressed) event journal on disk

Question 9 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The ESTEE architecture shown in Fig. 5.1 in unclear in terms of some of the inputs to the framework. E.g., allocated resources, target clustering configuration, etc. Could you explain in more detail how the inputs are described and what kind of inputs are expected? Also, in listing 5.1 there is no mention of target cluster, #CPUs, connections, etc. Could you explain more about how that information is input? Could you explain about the ESTEE simple “communication network model”.
> ”

Question 9 (assoc. prof. João Manuel Paiva Cardoso)

“

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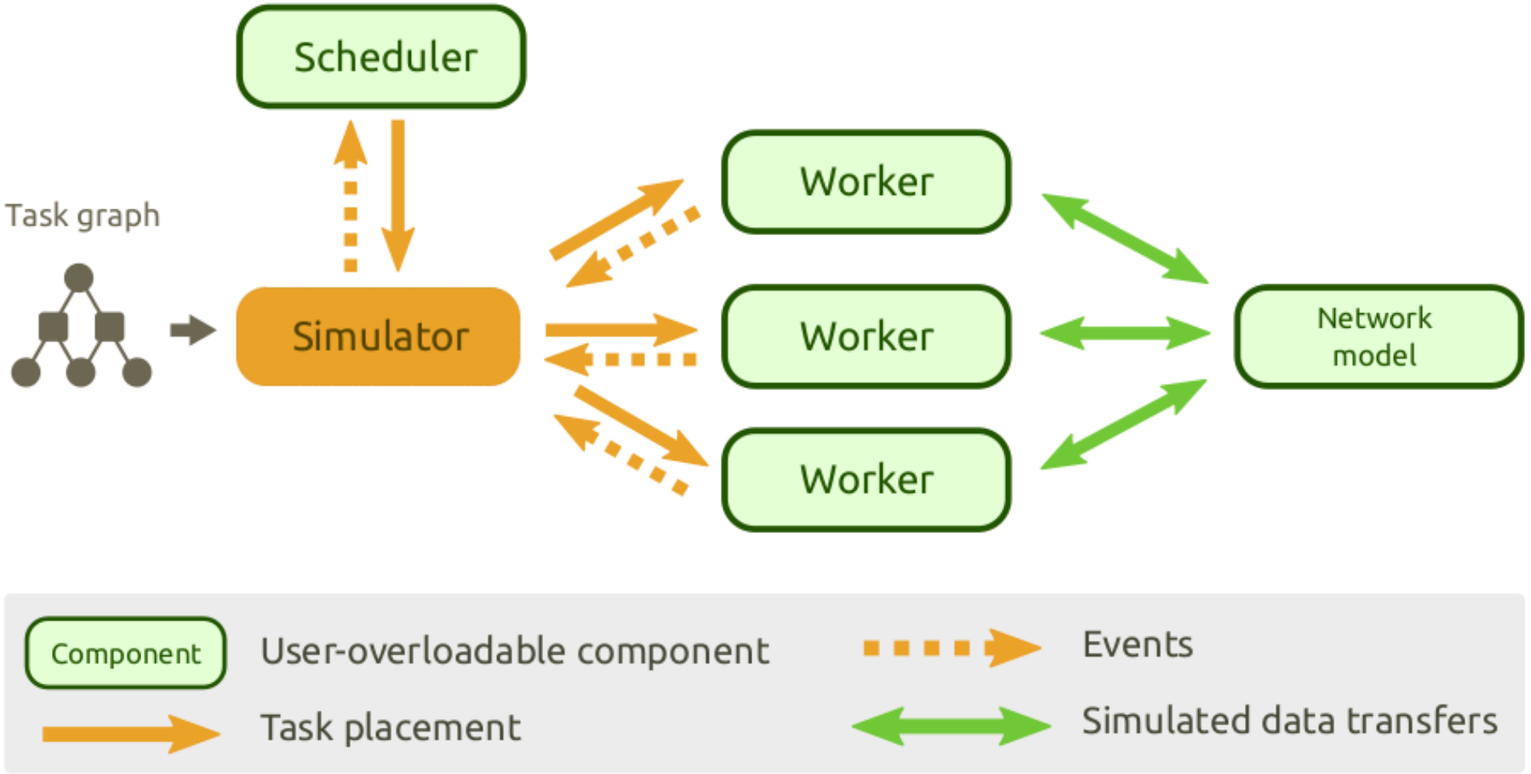

of the inputs
ration, etc.
hat kind of
cluster, #CPUs,
n is input?
model”.

”

Figure 5.1: ESTEE architecture

Question 9 (assoc. prof. João Manuel Paiva Cardoso)

“

```
# Create a task scheduler
scheduler = BlevelGtScheduler()

# Define cluster with 2 workers (1 CPU core each)
workers = [Worker(cpus=1) for _ in range(2)]

# Define MaxMinFlow network model (100MB/s bandwidth)
netmodel = MaxMinFlowNetModel(bandwidth=100)
```

”

Question 10 (assoc. prof. João Manuel Paiva Cardoso)

> “
> In terms of the scheduler, does the runtime system use updated execution times measured at runtime? And if so, how does it deal with that?
> ”

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- ESTEE does not do that, it is emulated by the *mean* imode

Question 10 (assoc. prof. João Manuel Paiva Cardoso)

> “
> In terms of the scheduler, does the runtime system use updated execution times measured at runtime? And if so, how does it deal with that?
> ”

- ESTEE does not do that, it is emulated by the *mean* imode
- Users decide task durations, so measuring them is not so important

Question 11 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Do the schedulers and the evaluation in subsection 5.2 deal with goals to use fewer CPUs as much as possible (part of the work selection strategy)? If so, how does it work?
> ”

Question 12 (assoc. prof. João Manuel Paiva Cardoso)

> “
> When considering different task graphs and the impact of them on the gap between the two network models in subsection 5.2, do you think that understanding the shape and main characteristics of the task graphs would help to improve scheduling decisions?
> ”

Question 12 (assoc. prof. João Manuel Paiva Cardoso)

> “When considering different task graphs and the impact of them on the gap between the two network models in subsection 5.2, do you think that understanding the shape and main characteristics of the task graphs would help to improve scheduling decisions?”

- Scheduling algorithms are heavily based on heuristics

Question 13 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Trends in terms of scheduler performance relative to b-level (in DASK and ESTEE, page 75) with different cluster configurations? Any thoughts about the effect of the task graph shapes/patterns on the accuracy of relative performance?
> ”

Question 13 (assoc. prof. João Manuel Paiva Cardoso)

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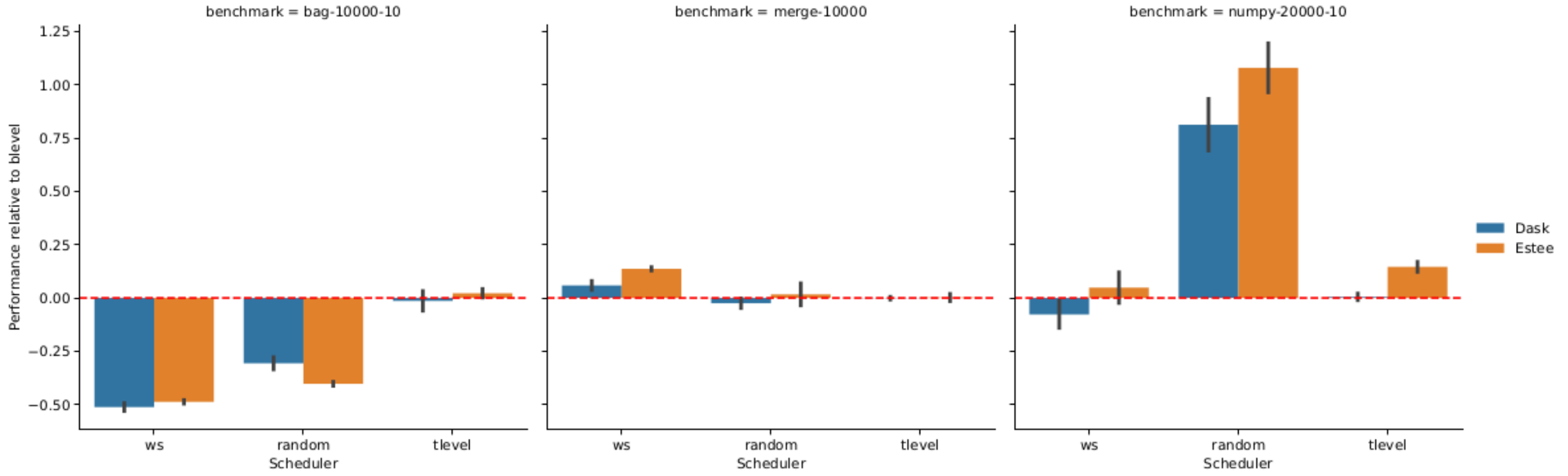

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”

Figure 5.7: Scheduler performance relative to *blevel* in DASK and ESTEE

Question 14 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Any task graph pattern/shape would be able to indicate when a scheduler is better than others and thus could be the one used? Use of the best for a particular task graph and cluster configuration.
> ”

Question 14 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Any task graph pattern/shape would be able to indicate when a scheduler is better than others and thus could be the one used? Use of the best for a particular task graph and cluster configuration.
> ”

- Graph shape *can* be a heuristic for selecting a scheduler

Question 15 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Any thoughts based on the experiments about the MSD (minimal scheduling delay) impact according to the scheduler and task graph? Long MSD implies less decisions of the scheduler but more knowledge (arrival of more task events).
> Does MSD imply similar effects on different information modes?
> ”

Question 15 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Any thoughts based on the experiments about the MSD (minimal scheduling delay) impact according to the scheduler and task graph? Long MSD implies less decisions of the scheduler but more knowledge (arrival of more task events). Does MSD imply similar effects on different information modes?
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- Configuring MSD is required to improve runtime performance

Question 15 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Any thoughts based on the experiments about the MSD (minimal scheduling delay) impact according to the scheduler and task graph? Long MSD implies less decisions of the scheduler but more knowledge (arrival of more task events). Does MSD imply similar effects on different information modes?
> ”

- Configuring MSD is required to improve runtime performance
- Unclear how to predict its effect on scheduling (heuristics)

Question 16 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The task runtime optimization evaluations would benefit from the knowledge of optimal scheduling. This could be very important to understand the potential for further improvements in terms of the actual results with heuristics.
> Do you see an experimental way to know those optimal results?
> ”

Question 16 (assoc. prof. João Manuel Paiva Cardoso)

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> Do you see an experimental way to know those optimal results?
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- Complex benchmarks generated from real-world numpy/pandas code

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> “
> The task runtime optimization evaluations would benefit from the knowledge of optimal scheduling. This could be very important to understand the potential for further improvements in terms of the actual results with heuristics.
> Do you see an experimental way to know those optimal results?
> ”

- Complex benchmarks generated from real-world numpy/pandas code
- NP-hard to get optimal scheduling (brute-force)

Question 17 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The limitation of tasks in pure Python and on the constraint to workers behave in a single-threaded fashion, … may have a high overhead. Any thoughts on that overhead and when it is adequate to circumvent the limitation? Any thoughts about the main conclusions regarding I/O-bound vs compute-bound benchmarks?
>
> ”

Question 17 (assoc. prof. João Manuel Paiva Cardoso)

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- Each worker introduces scheduling and communication overhead

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>
> ”

- Each worker introduces scheduling and communication overhead
- 'Time spent in Python' vs 'Time spent in C/C++ or I/O or other program'

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>
> ”

- Each worker introduces scheduling and communication overhead
- 'Time spent in Python' vs 'Time spent in C/C++ or I/O or other program'
- Python 3.13+ has support for running without GIL

Question 18 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Fig. 6.2 and 6.3 (page 86) show the overhead per task when increasing the number of tasks and using two benchmarks (“merge” and “merge-25000”). Are the results similar to other benchmarks? Why the use of these benchmarks and the ones in Fig. 6.4 and 6.5 (page 87) for studying the scaling of DASK and the effect of GIL?
> ”

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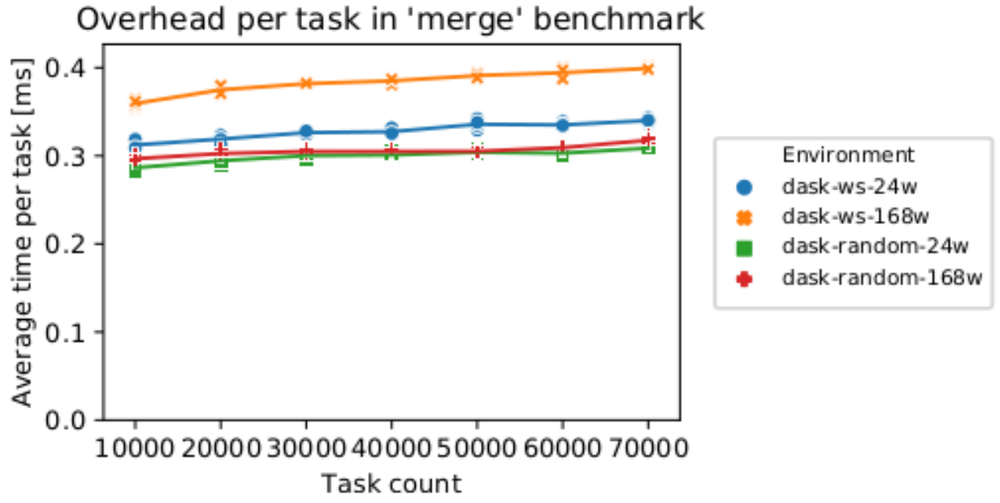

Figure 6.2: Overhead per task in DASK with an increasing number of tasks.

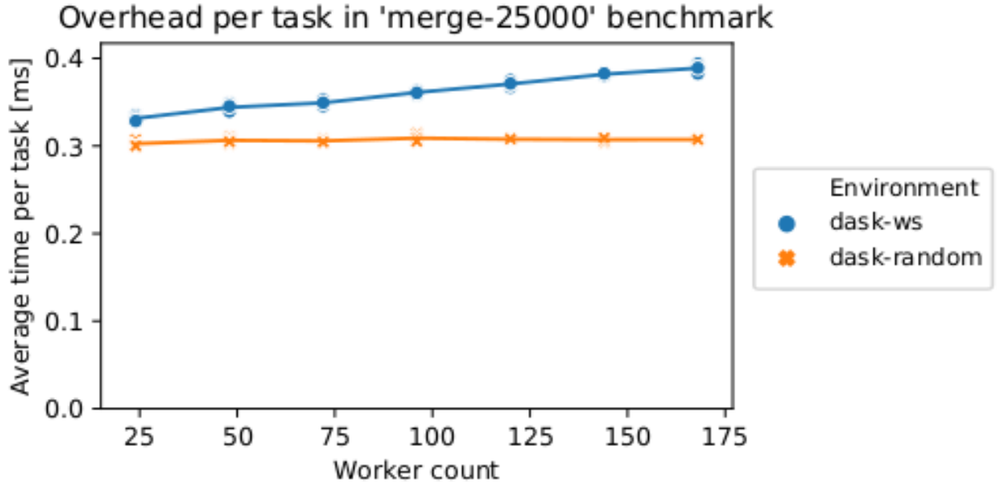

Figure 6.3: Overhead per task in DASK with an increasing number of workers.

Question 18 (assoc. prof. João Manuel Paiva Cardoso)

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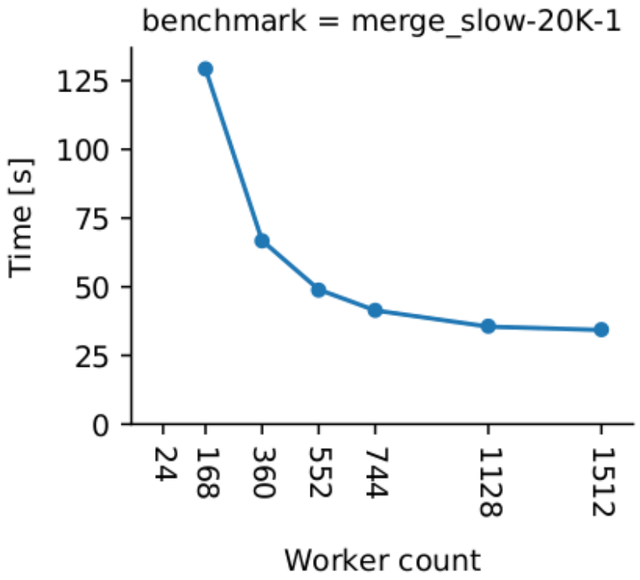

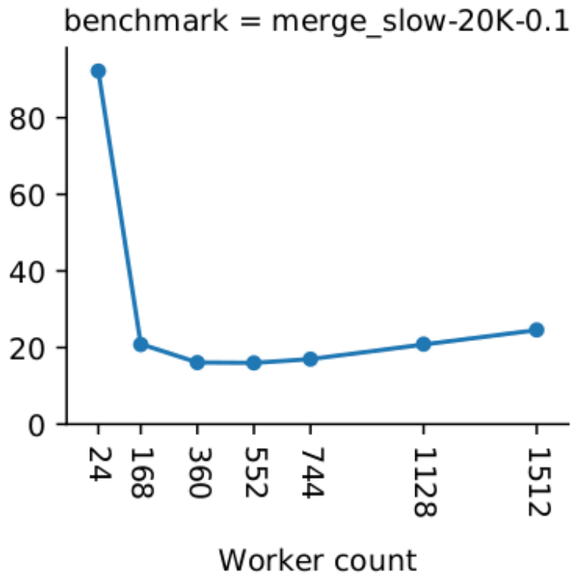

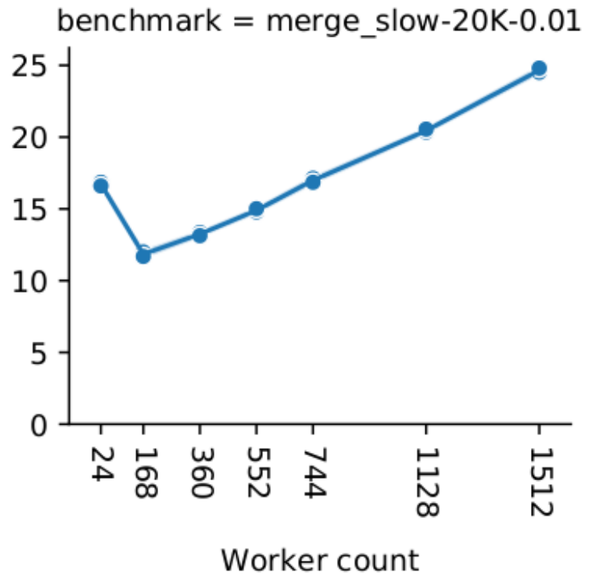

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Figure 6.4: Strong scaling of Dask with different task durations (1000 ms, 100 ms and 10 ms).

Question 18 (assoc. prof. João Manuel Paiva Cardoso)

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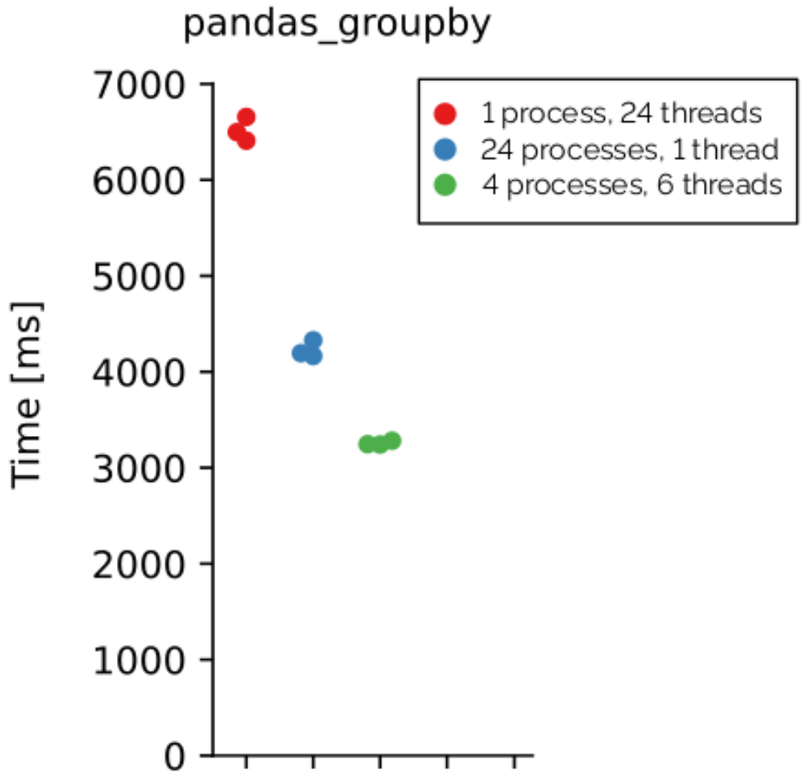

Figure 6.5: Effect of GIL on the performance of the *pandas_groupby* benchmark

Question 19 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The manual tuning of worker configuration (impact of worker per core and the non-optimal scalability of DASK) for some workflows seems very important to improve performance. Any idea if this can be statically determined?
> ”

Question 19 (assoc. prof. João Manuel Paiva Cardoso)

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> ”

- Very difficult to determine, can differ task by task

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> “
> The manual tuning of worker configuration (impact of worker per core and the non-optimal scalability of DASK) for some workflows seems very important to improve performance. Any idea if this can be statically determined?
> ”

- Very difficult to determine, can differ task by task
- Affects the configuration of the cluster

Question 20 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Any thoughts about providing schedulers the worker network connections? Do you see a relevant impact on RSDS?
> ”

Question 21 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Since RSDS does not implement all DASK message types, do you see in future plans their integration to RSDS, or are there technical challenges that do not justify their integration?
> ”

Question 21 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Since RSDS does not implement all DASK message types, do you see in future plans their integration to RSDS, or are there technical challenges that do not justify their integration?
> ”

- Some messages are Python specific

Question 21 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Since RSDS does not implement all DASK message types, do you see in future plans their integration to RSDS, or are there technical challenges that do not justify their integration?
> ”

- Some messages are Python specific
- 'Run this Python code on the server'

Question 22 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Why do the schedulers (ws and random) integrated in RSDS do not include a list-scheduling or an ALAP scheduling scheme?
> ”

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> “
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> ”

- Work-stealing is list scheduling (B-level) + balancing between workers

Question 22 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Why do the schedulers (ws and random) integrated in RSDS do not include a list-scheduling or an ALAP scheduling scheme?
> ”

- Work-stealing is list scheduling (B-level) + balancing between workers
- We focused on runtime optimization

Question 23 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The conclusion that the improved performance of RSDS with ws is caused by better runtime efficiency and not by better schedules seems to result from the large overhead of the DASK implementation. (page 93)
> Could you comment on this?
> ”

Question 23 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The conclusion that the improved performance of RSDS with ws is caused by better runtime efficiency and not by better schedules seems to result from the large overhead of the DASK implementation. (page 93)
> Could you comment on this?
> ”

- RSDS/ws vs Dask/ws: 1.66x

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> Could you comment on this?
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- RSDS/ws vs Dask/ws: 1.66x
- Dask/random vs Dask/ws: 0.95x

Question 23 (assoc. prof. João Manuel Paiva Cardoso)

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> The conclusion that the improved performance of RSDS with ws is caused by better runtime efficiency and not by better schedules seems to result from the large overhead of the DASK implementation. (page 93)
> Could you comment on this?
> ”

- RSDS/ws vs Dask/ws: 1.66x
- Dask/random vs Dask/ws: 0.95x
- RSDS/random vs Dask/ws: 1.41x

Question 24 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The results presented in Fig. 6.11, page 96, seem to indicate a greater dependence of DASK to #workers (its “performance is reduced significantly with each additional worker”) than RSDS. Could you elaborate on that? Could part of the overhead reduction of RSDS over DASK, besides the implementation used, be because of the much simpler ws scheduling scheme used by RSDS when compared to DASK?
>
> ”

Question 24 (assoc. prof. João Manuel Paiva Cardoso)

“

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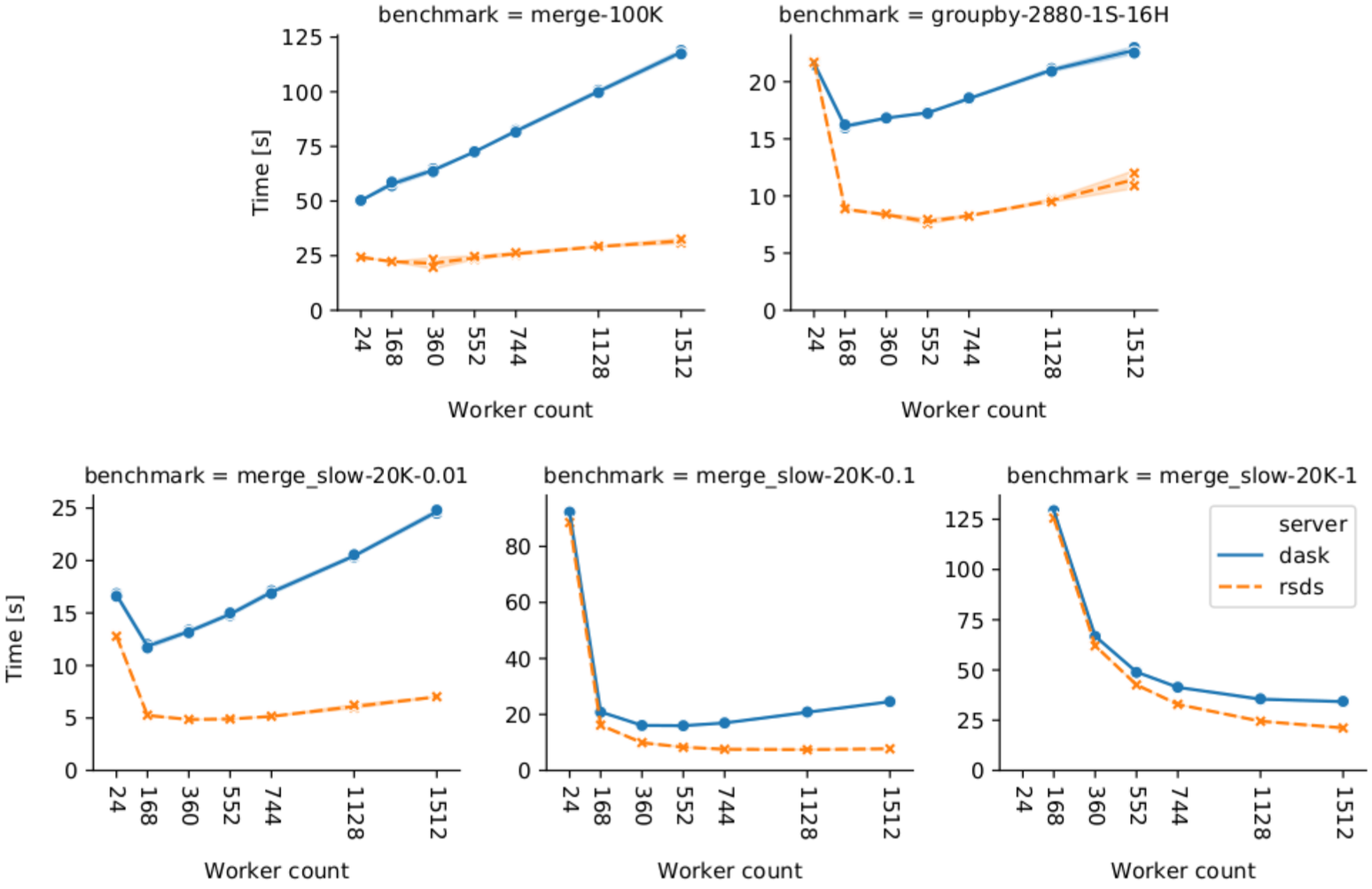

Figure 6.11: Strong scaling of RSDS vs Dask on selected task graphs

Question 25 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Do the overheads of DASK and RSDS for each task depend on the number of workers and tasks in the task graph? What is the reason for the significant overhead increase in RSDS with some of the benchmarks (Fig. 6.14, page 98)?
> ”

Question 25 (assoc. prof. João Manuel Paiva Cardoso)

“

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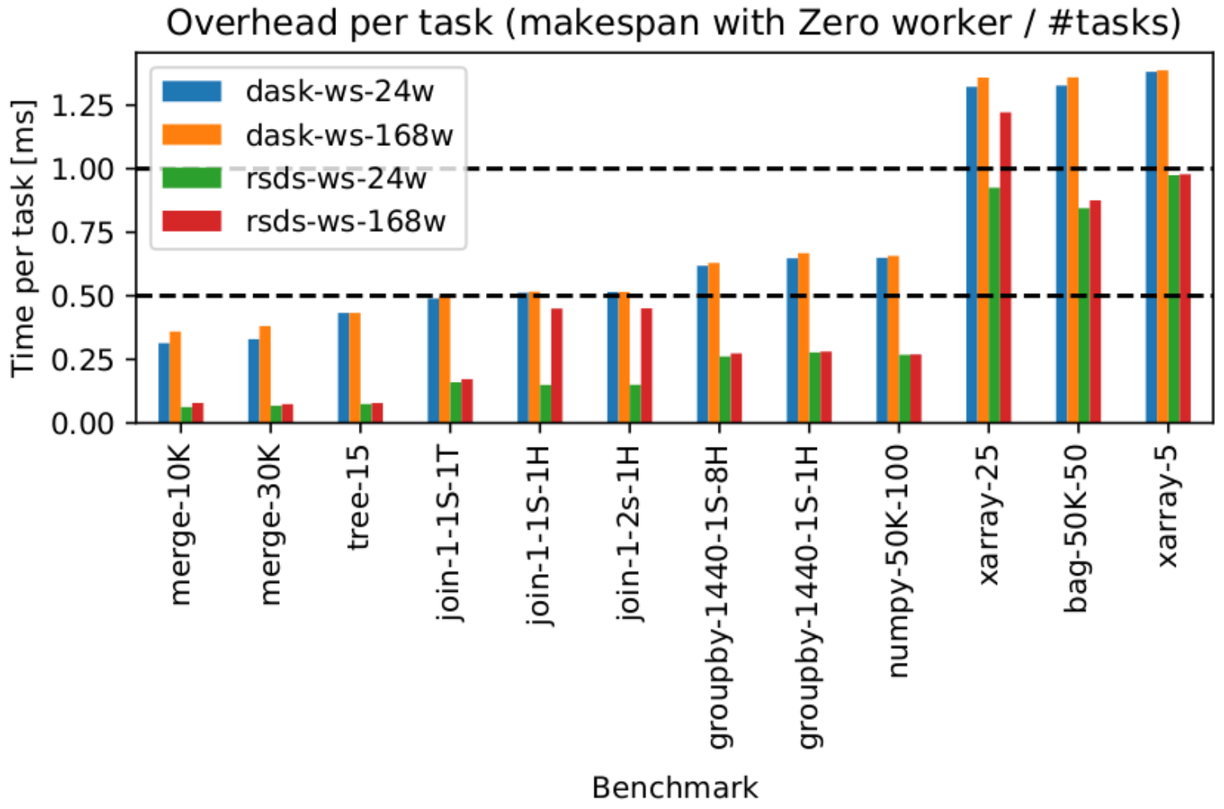

number
significant
4, page 98)?

”

Figure 6.14: Overhead per task for various cluster sizes and benchmarks

Question 26 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The thesis mentions that task graphs are represented in a compressed format, but that format is not fully described. Could you elaborate on this?
> ”

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- Representation of a task x number of tasks

Question 26 (assoc. prof. João Manuel Paiva Cardoso)

> “The thesis mentions that task graphs are represented in a compressed format, but that format is not fully described. Could you elaborate on this?”

- Representation of a task x number of tasks
- Currently used only for task arrays (DAGs without dependencies)

Question 26 (assoc. prof. João Manuel Paiva Cardoso)

> “
> The thesis mentions that task graphs are represented in a compressed format, but that format is not fully described. Could you elaborate on this?
> ”

- Representation of a task x number of tasks
- Currently used only for task arrays (DAGs without dependencies)
- Could be extended to support also task dependencies (Dask does this)

Question 27 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Why the fractional resource requirements in HYPERQUEUE are not defined as integer percentages and need to use fixed-point representations?
> ”

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> ”

- Fixed-point arithmetic is essentially integer percentages

Question 27 (assoc. prof. João Manuel Paiva Cardoso)

> “
> Why the fractional resource requirements in HYPERQUEUE are not defined as integer percentages and need to use fixed-point representations?
> ”

- Fixed-point arithmetic is essentially integer percentages
- Floating point operations have precision problems

Question 28 (assoc. prof. João Manuel Paiva Cardoso)

> “
> It is interesting that HYPERQUEUE showed unnecessary tuning on the number of used nodes and workers, and number of tasks and task durations, as opposite of DASK has shown. What is the main reason for this?
> ”

Question 28 (assoc. prof. João Manuel Paiva Cardoso)

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> ”

- No GIL

Question 28 (assoc. prof. João Manuel Paiva Cardoso)

> “
> It is interesting that HYPERQUEUE showed unnecessary tuning on the number of used nodes and workers, and number of tasks and task durations, as opposite of DASK has shown. What is the main reason for this?
> ”

- No GIL
- Single node = single worker, which manages all node resources

Question 29 (assoc. prof. João Manuel Paiva Cardoso)

> “
> How do you see the possible support of HYPERQUEUE to data transfers directly between tasks? And to streaming and task pipelining support?
> ”

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- This is currently work-in-progress

Question 29 (assoc. prof. João Manuel Paiva Cardoso)

> “How do you see the possible support of HYPERQUEUE to data transfers directly between tasks? And to streaming and task pipelining support?”

- This is currently work-in-progress
- Need to figure out task completion semantics and fault tolerance