# Raythena: A Vertically Integrated Scheduler for ATLAS Applications on Heterogeneous Distributed Resources

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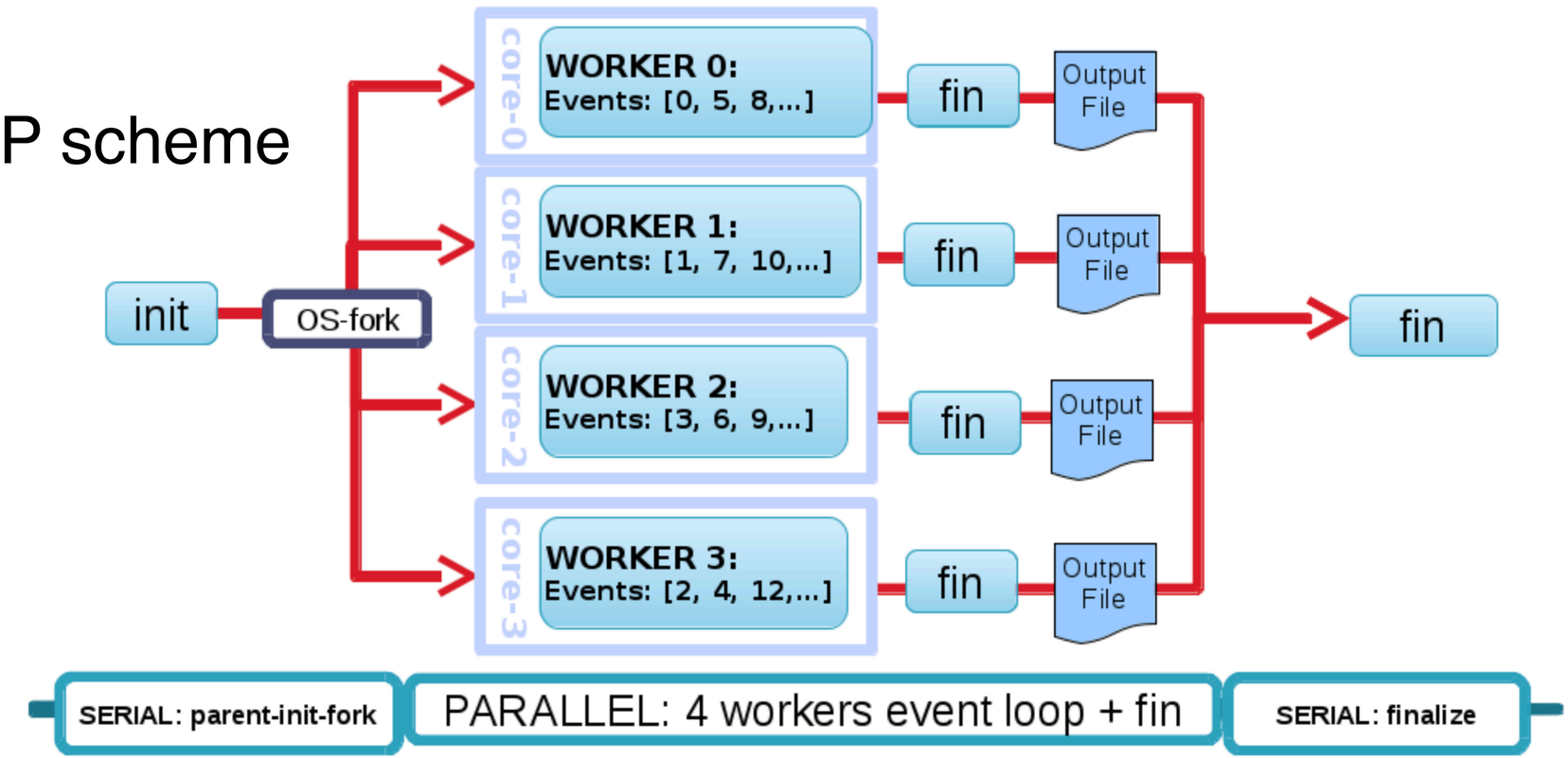
# Introduction

- We are exploring the applicability of a modern *distributed execution framework* for ATLAS workflows— Ray[1],
- **Distributed execution frameworks** allows the user to seamlessly transform a single-node application to run efficiently on a cluster of nodes or on a (heterogeneous) HPC,
- As a proof-of-concept, we present a Ray-based prototype of the ATLAS Event Service,
- Advantages of using Ray:
  - Ray is widely used by the broader community and centrally maintained. Using Ray would eliminate the need of supporting some of the ATLAS home-built software,
  - Shown to be scalable on HPCs, lightweight and easy to install (e.g. as a module),
  - It would establish a generic and modular workflow that could be used on all HPCs as a single solution.

# Athena framework in ATLAS

- Athena is the main software framework in ATLAS used for all data analysis steps,
- In this application we are using ‘AthenaMP’, the multi-process version of Athena,
- In the Event Service mode, input events are provided on demand by an external application. The number of input events does not need to be known in advance.

AthenaMP scheme

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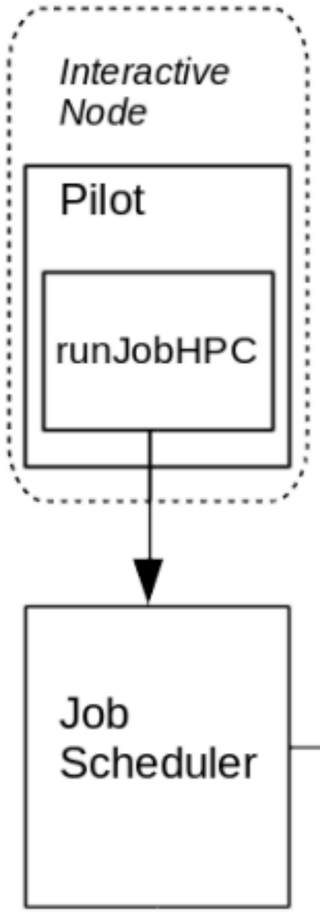
# Current scheduling on HPCs (i.e. the Yoda Workflow)

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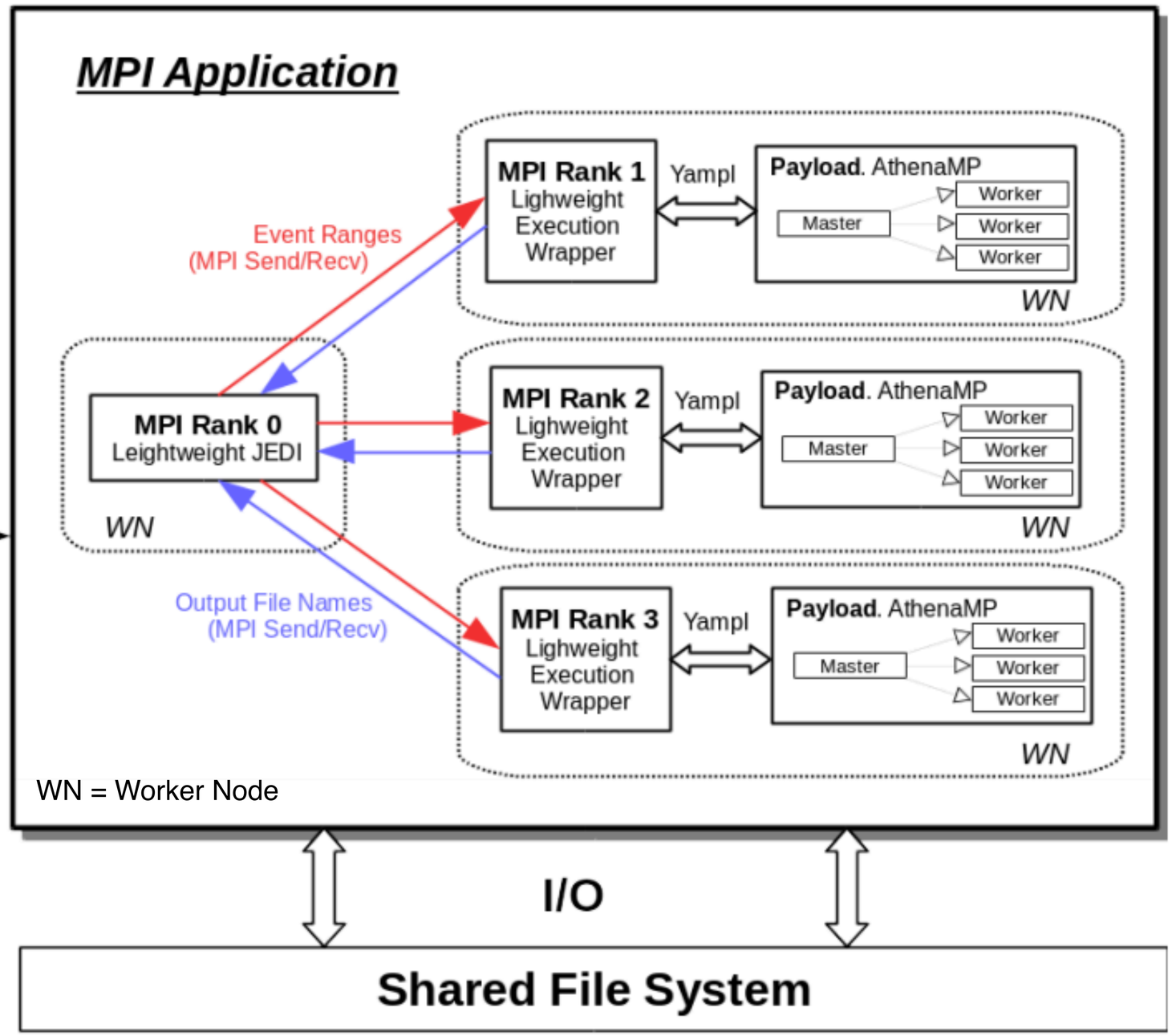
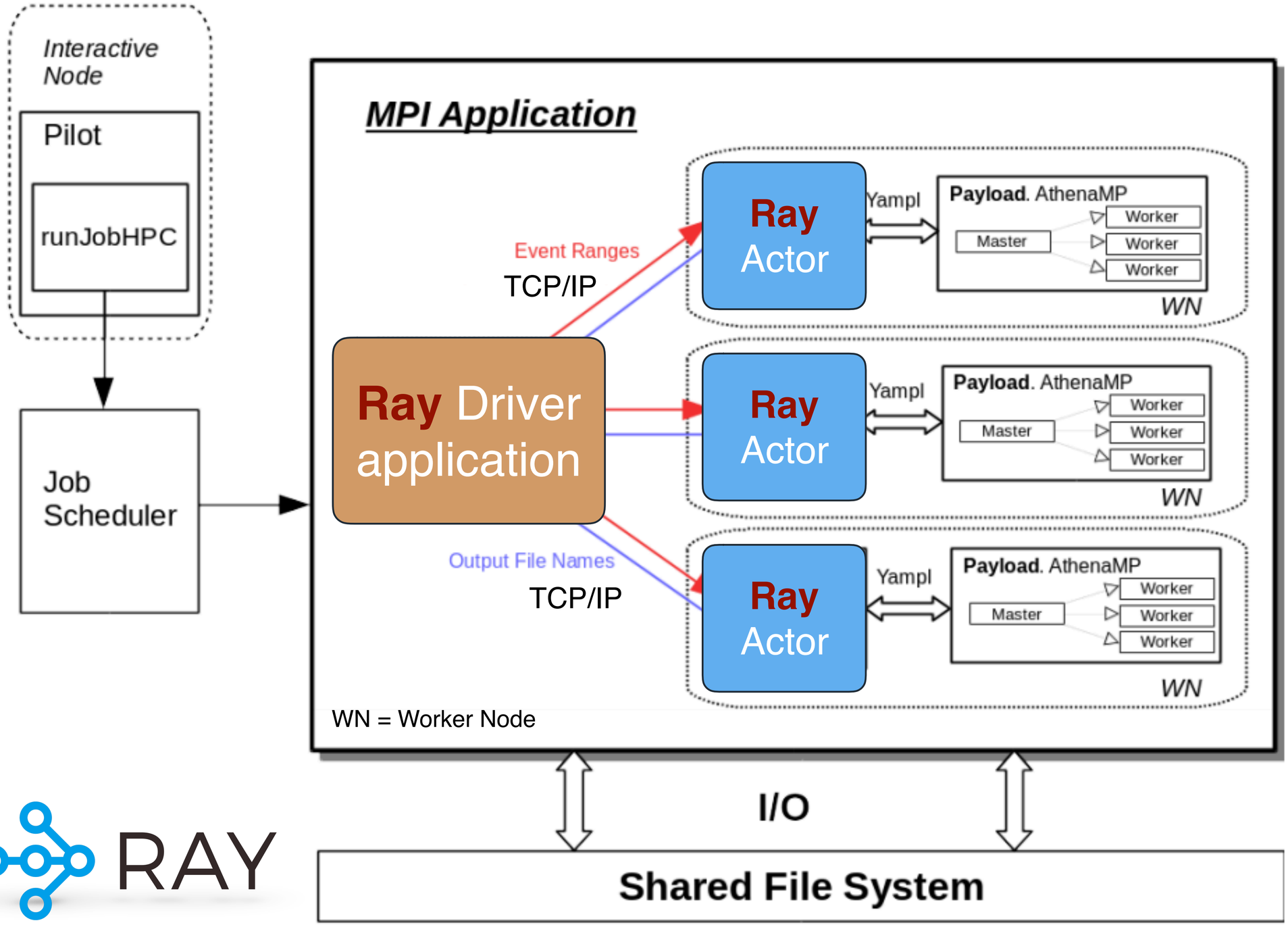


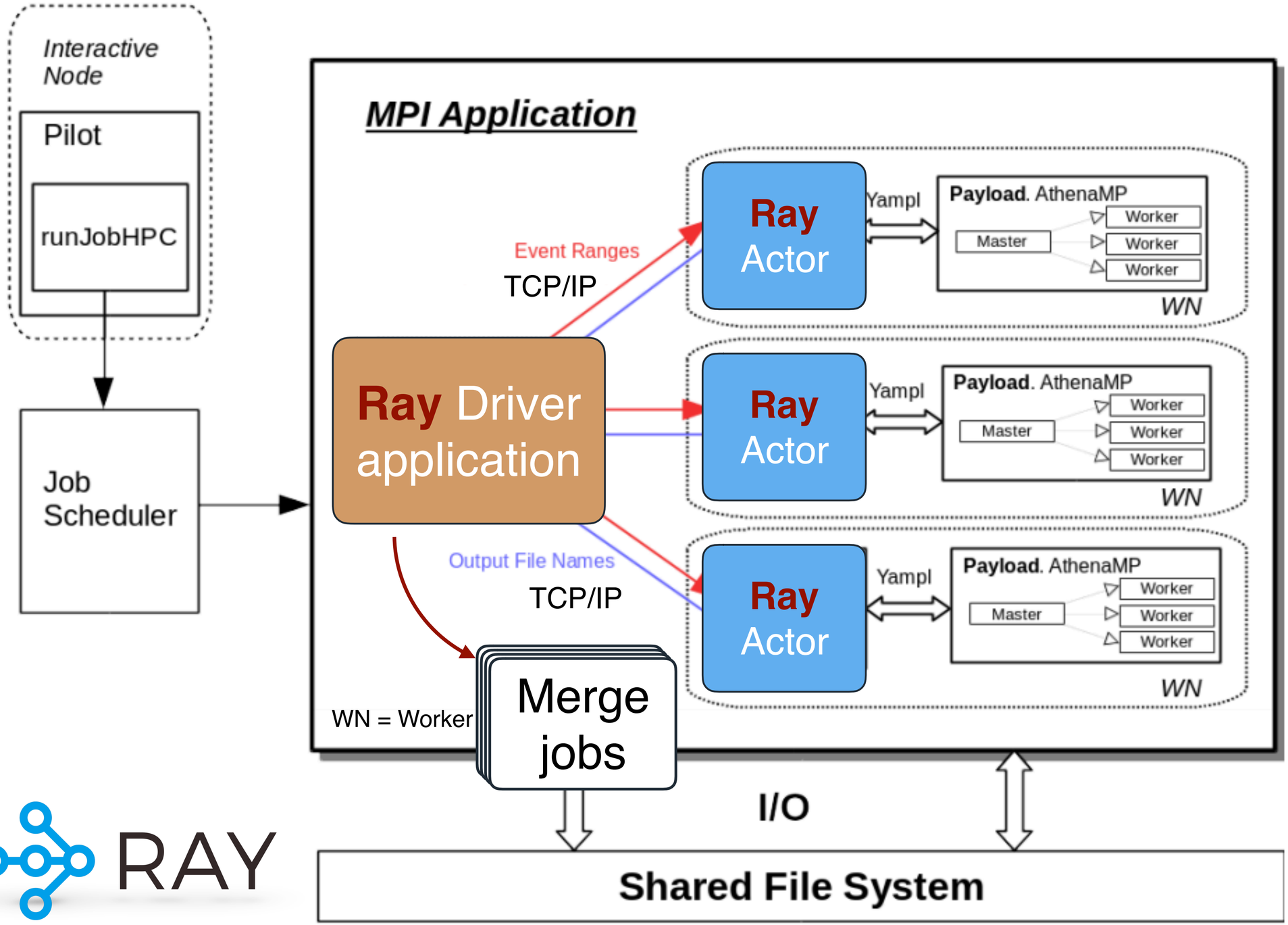

Currently composed of many different communication layers developed ‘in-house’ which are difficult to maintain with a limited person power.

# Ray-based ATLAS Event Service




Since Ray takes care of all communication between nodes and orchestration of workload, the Event Service application becomes more manageable and more modular.

# Ray-based ATLAS Event Service




RAY

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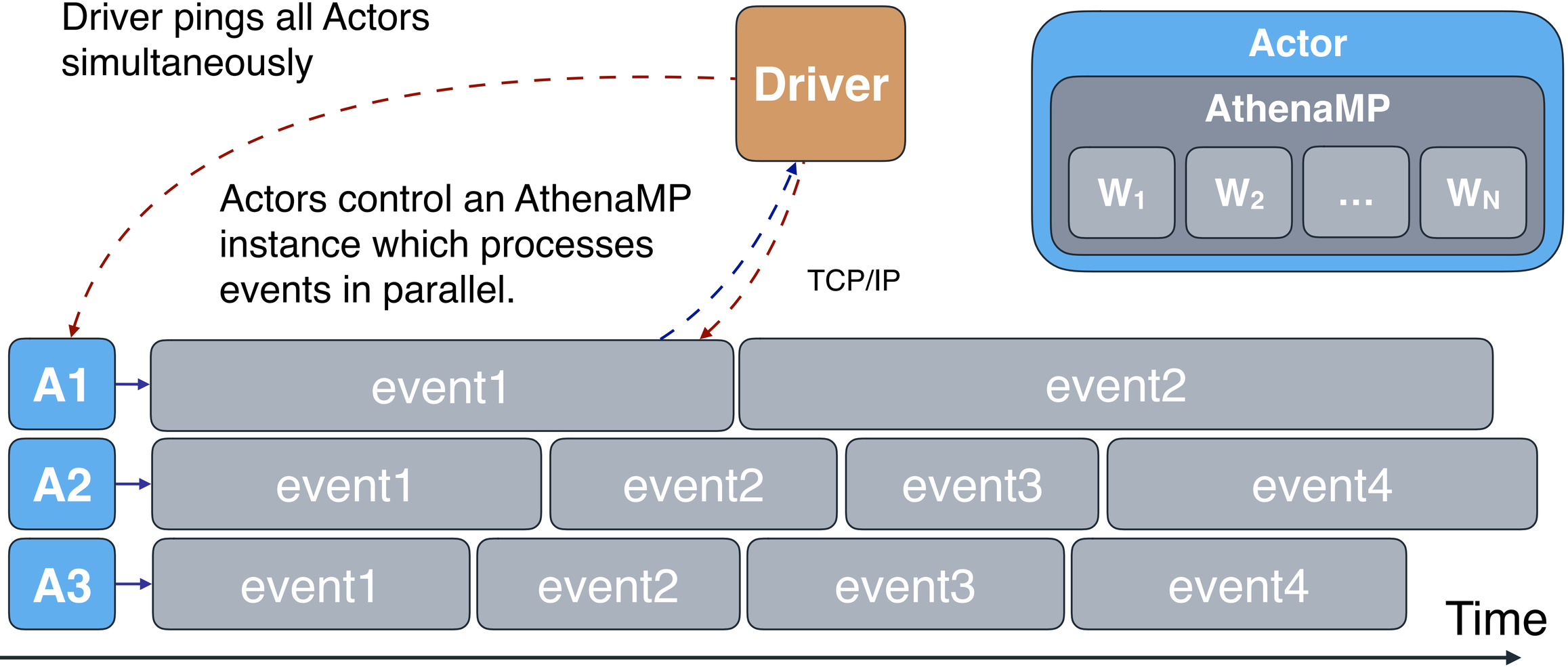
Additional features such as fault detection or ‘on-the-fly’ merging can be easily implemented in the driver application.

# Asynchronous communication between the Driver and Actors

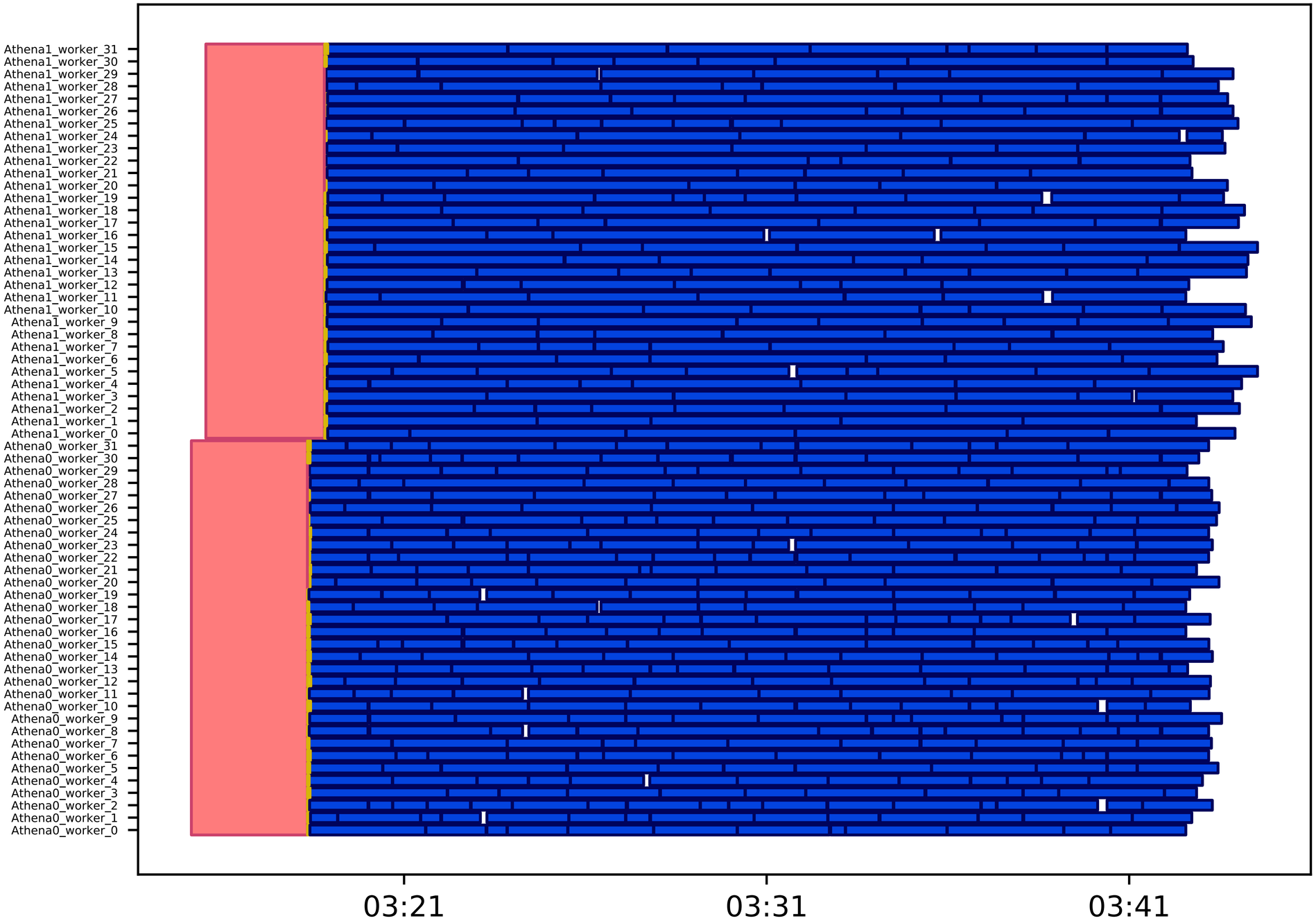
- Asynchronous communication is implemented in a few 100 python lines using Ray explicit parallelism expressions,
- Actors independently communicate with the AthenaMP instance and report back to the driver only when an event was processed and new input is needed.



# Working example on Cori at NERSC

- Successfully tested the Raythena workflow on Cori **Haswell** and **KNL** nodes at NERSC,
- Test jobs were ATLAS Geant4 simulation jobs that take ~few min. per event,
- Largest test that we tried so far:
  - 60 Haswell nodes with 32 cores each,
  - Processed 100k events in total and spawned merge jobs every 100 events to form 1000 merged output files,
- No bottlenecks found so far in Ray.

# Close-up — two AthenaMP instances on Haswell nodes




AthenaMP Initialization

Worker

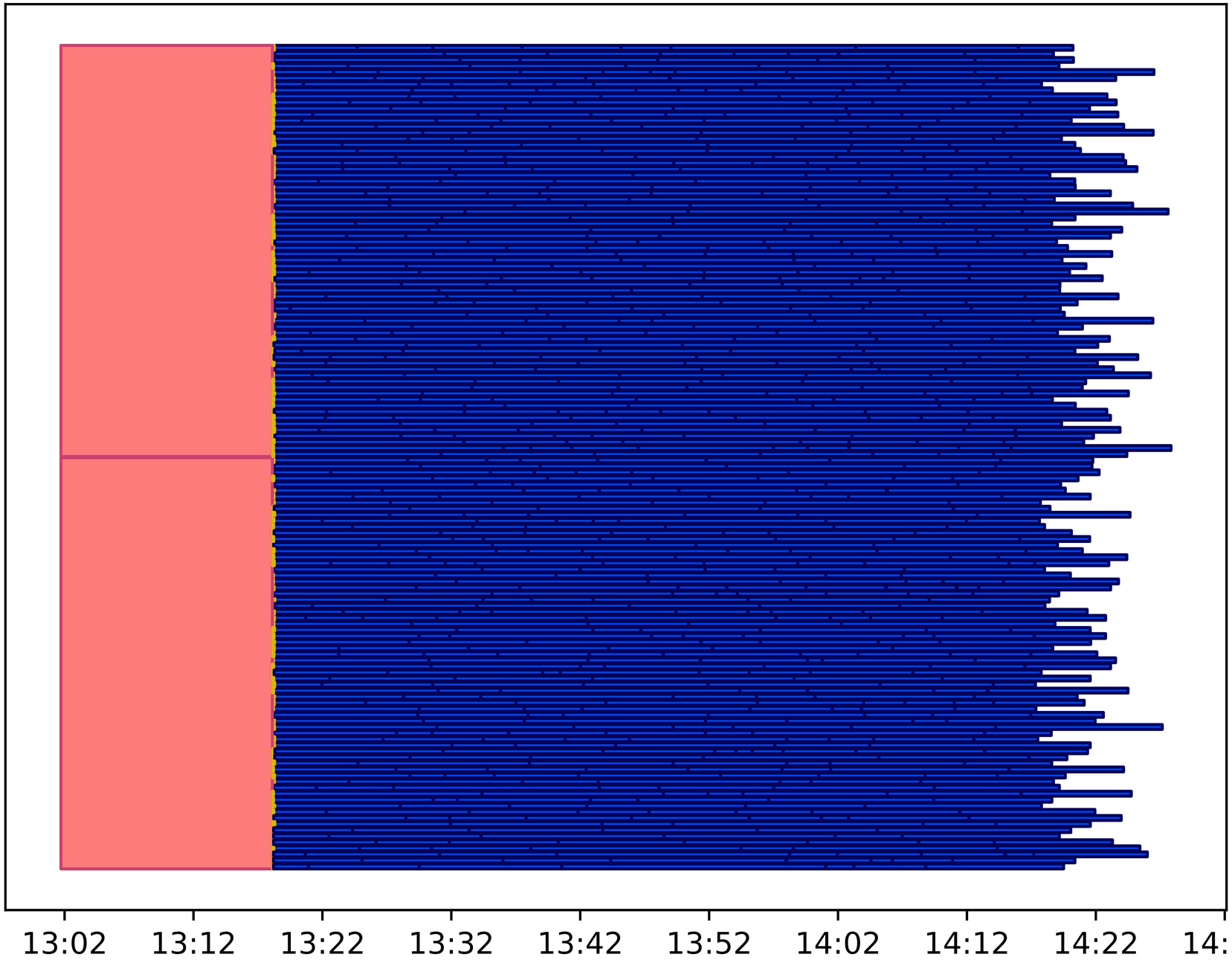
Event Processing

Worker Initialization

[Cori Haswell Nodes](#)
- 32 cores / node

wall time

# Close-up — two AthenaMP instances on KNL nodes




AthenaMP Initialization

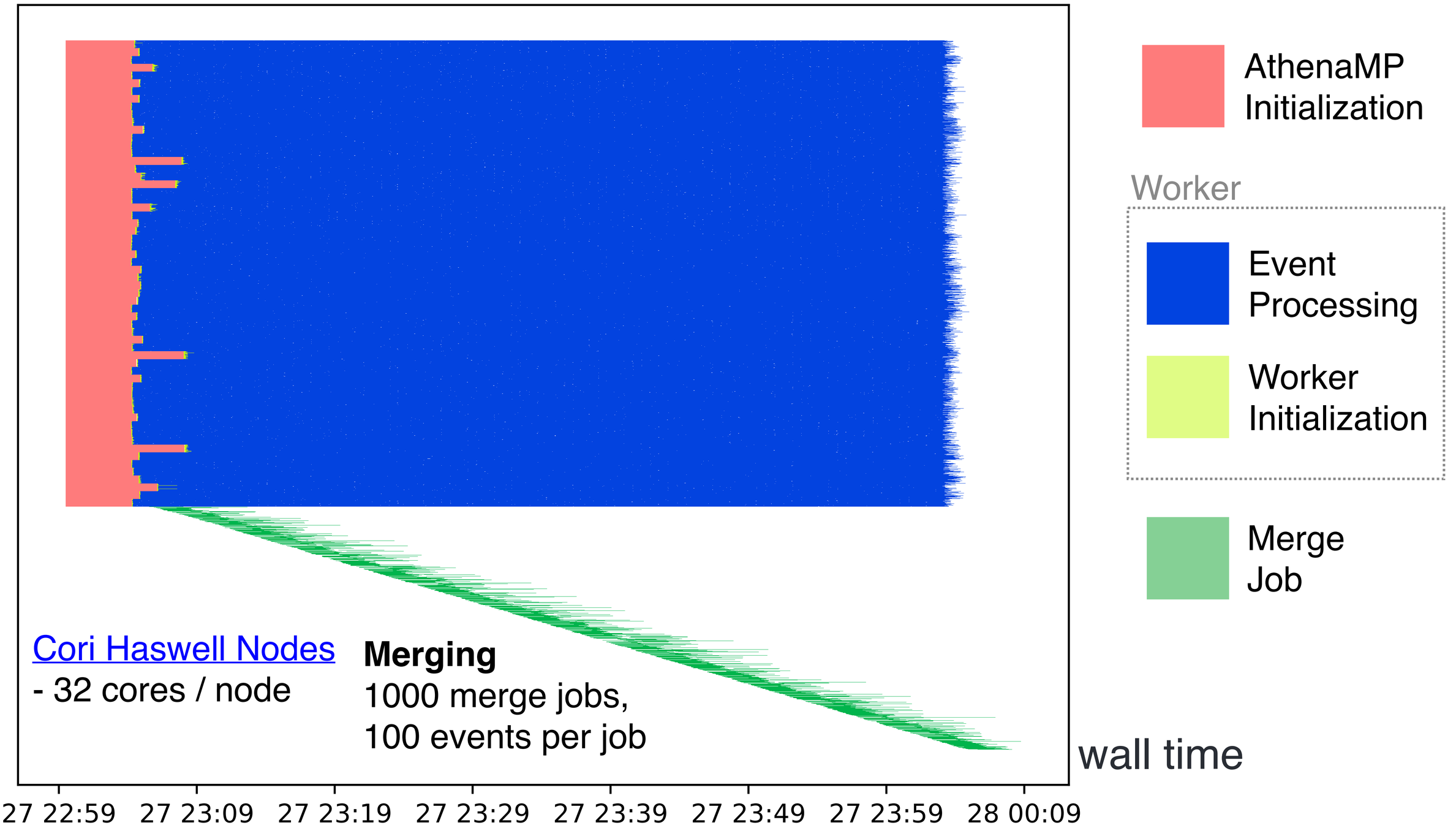
Worker

Event Processing

Worker Initialization

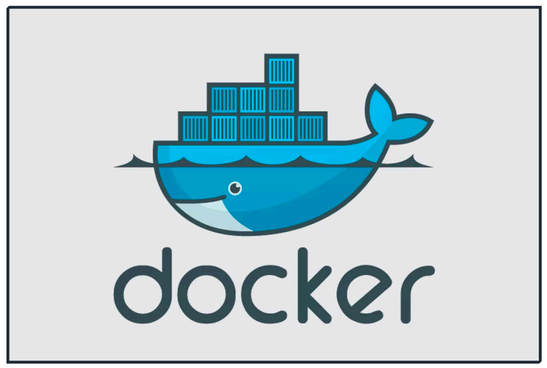
[Cori KNL Nodes]
- 68 cores / node

# Large Haswell job example (60 AthenaMP instances, 100k events)



# Raythena running scheme

```
$ sbatch –image mmuskinj/some-ray-image –module=cvmfs
```

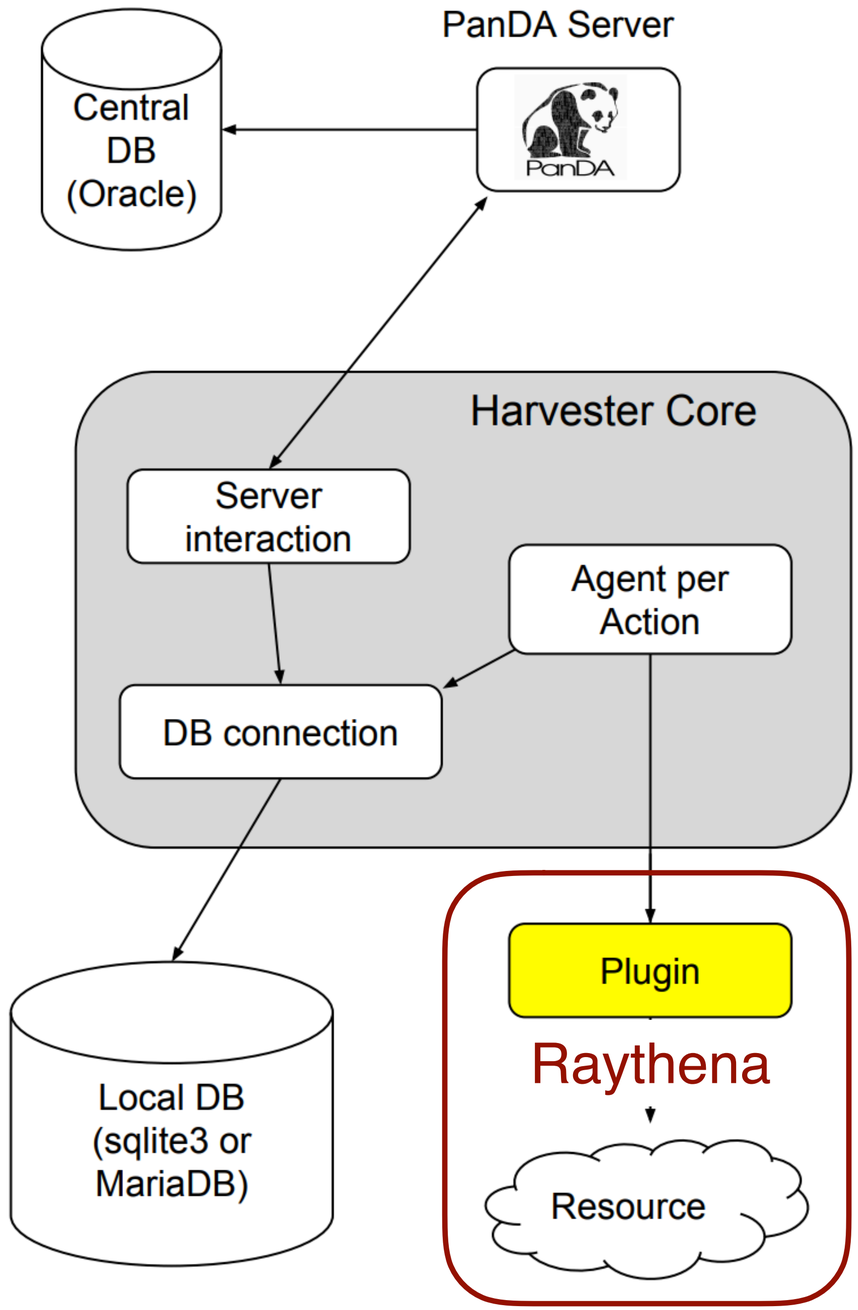



```
$ shifter ./ray_start_head.sh
$ srun shifter ./ray_start_other.sh &
$ shifter ./run_raythena.sh
```

- Ray, Raythena, and Athena are all running in a container on all nodes,
- Can be ported to other HPCs without too much effort.

# Raythena plans for Run 3

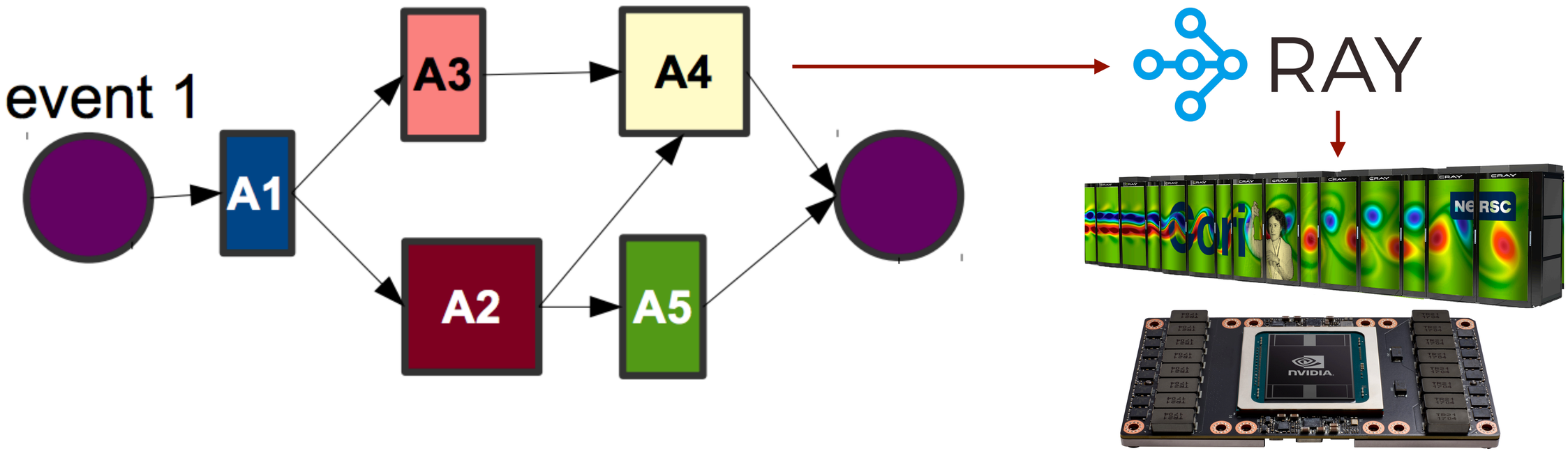
- We are working towards using Raythena as the default job orchestrating application on HPCs in Run 3,
- Raythena batch jobs will be spawned by Harvester— an application connected to the PanDA server,
- PanDA is the ATLAS Production and Distributed Analysis system use for all production job submission,
- More details given by Paul Nilsson today: https://indico.cern.ch/event/773049/contributions/3473371/.




https://cds.cern.ch/record/2625435/

# Digging deeper into Athena / Gaudi

- The long-term project is to interface Athena/Gaudi algorithms directly to Ray for a much finer control over scheduling the workload,
- This would replace the current event loop with Ray and enable scheduling of a single event across several nodes,
- Data needed by the algorithms is provided by Ray's Global Control Store (GCS),
- Maximize throughput by more efficient/tailored scheduling of algorithms to computing resources (e.g., CPU vs GPU).



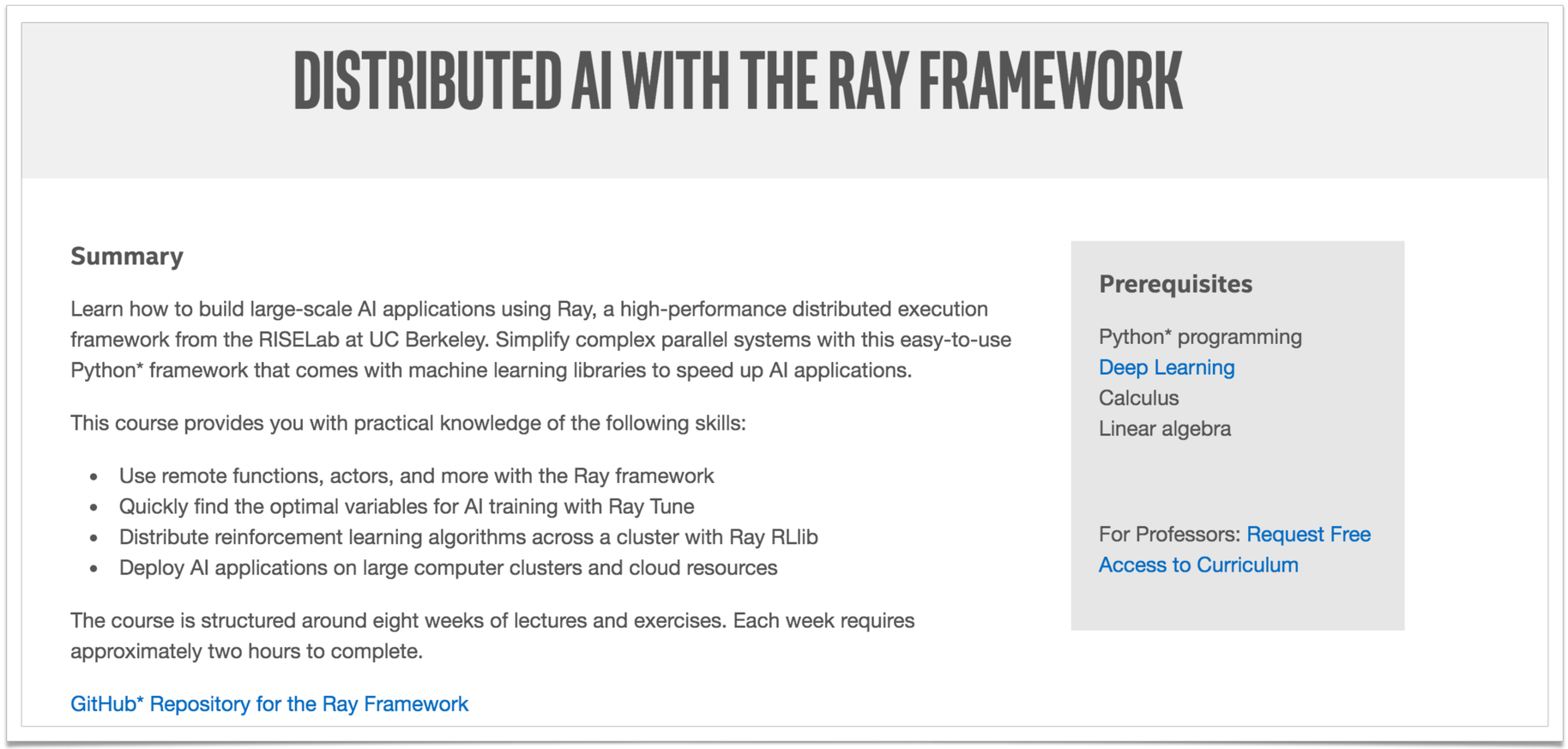
# Summary

- We are exploring the applicability of a distributed execution framework (Ray) for ATLAS workflows,
- We have demonstrated a stand-alone prototype of a Ray-based ATLAS Event Service,
  - Shown to be scalable on Cori Haswell and KNL nodes,
  - Runs entirely from containers and is portable to other HPCs,
  - Plan is to use it as the default intermediate layer between Harvester and AthenaMP processes on compute nodes in Run 3 for large-scale production jobs.
- Longer-term-plan is to divide the ATLAS workflow into base components (Algorithms) and interface them directly to Ray.

# BACKUP

# Ray documentation and tutorials

- Ray has a very rich documentation hosted on readthedocs:
  - https://ray.readthedocs.io/en/latest/index.html,
- Hands-on tutorials with exercises available in form of jupyter notebooks,
- Since Feb 2019, Intel hosts an 8-week course about distributed AI computation with Ray: https://software.intel.com/en-us/ai/courses/distributed-AI-ray.



DISTRIBUTED AI WITH THE RAY FRAMEWORK

**Summary**

Learn how to build large-scale AI applications using Ray, a high-performance distributed execution framework from the RISELab at UC Berkeley. Simplify complex parallel systems with this easy-to-use Python* framework that comes with machine learning libraries to speed up AI applications.

This course provides you with practical knowledge of the following skills:

- Use remote functions, actors, and more with the Ray framework
- Quickly find the optimal variables for AI training with Ray Tune
- Distribute reinforcement learning algorithms across a cluster with Ray RLlib
- Deploy AI applications on large computer clusters and cloud resources

The course is structured around eight weeks of lectures and exercises. Each week requires approximately two hours to complete.

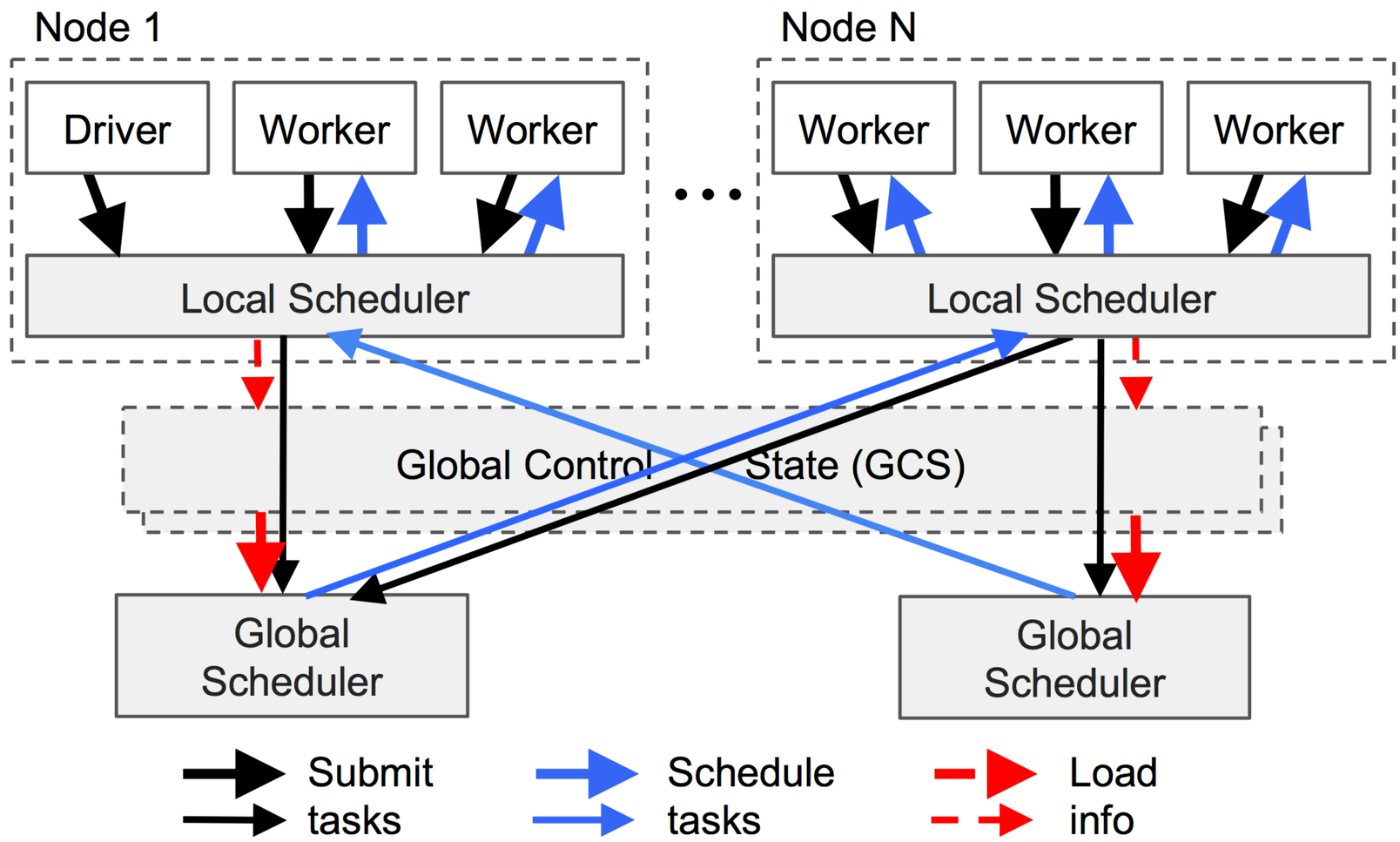
GitHub* Repository for the Ray Framework

**Prerequisites**

Python* programming
Deep Learning
Calculus
Linear algebra

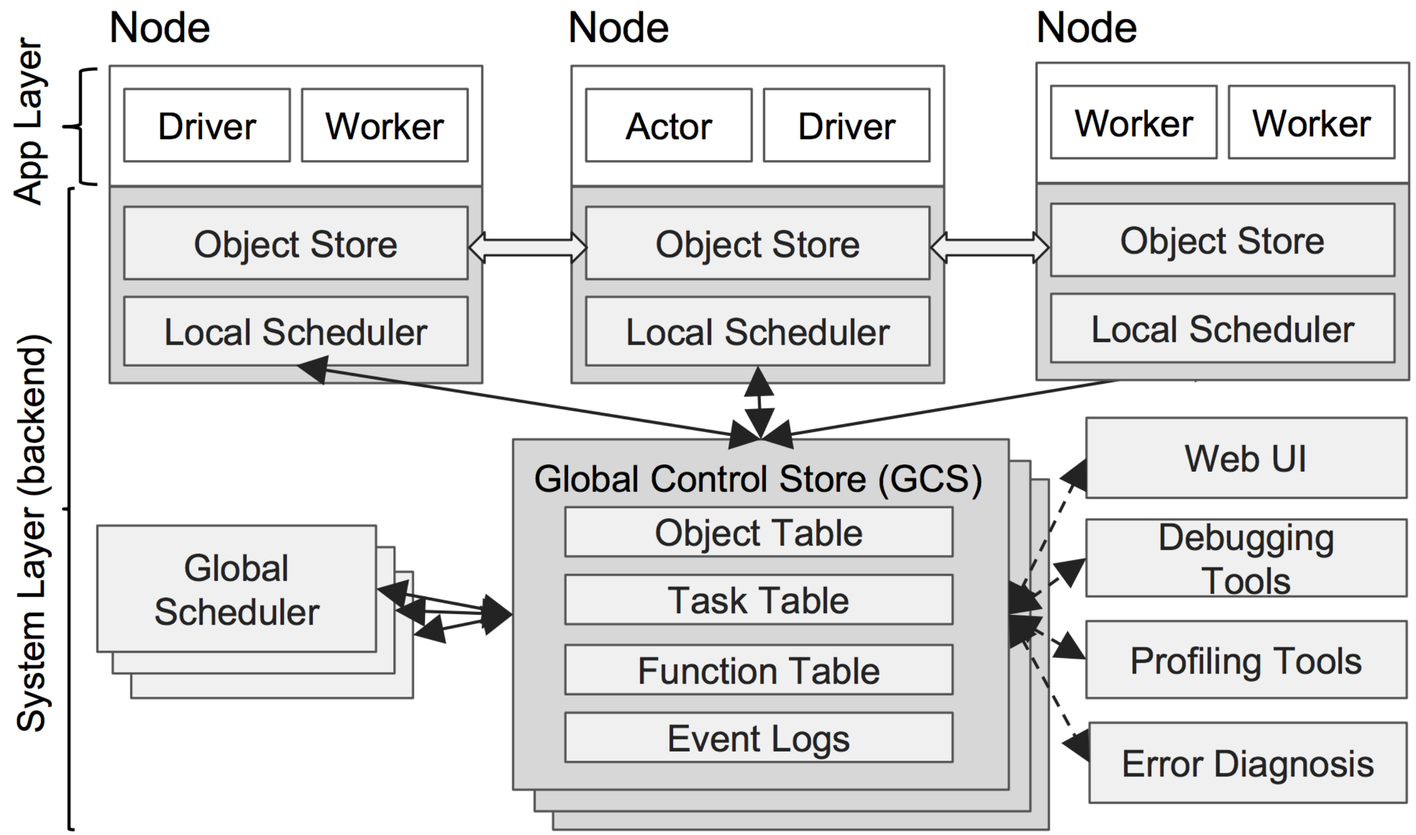
For Professors: Request Free Access to Curriculum

- One driver application (running on any compute node) controls all nodes in a cluster (HPC) that are connected via TCP to a redis server,
- Tasks are first scheduled locally (Local Scheduler) if resources are available, otherwise they are scheduled globally via the Global Scheduler.



# Ray Application Layer

- Ray maintains three types of processes:
  - *Driver*: a process executing the user program,
  - *Worker*: a stateless process that executes tasks invoked by the driver or another worker. Workers are started automatically and execute tasks serially without maintaining a local state,
  - *Actor*: a stateful process that executes only the method it exposes. They execute methods serially and each method depends on the state resulting from the previous execution.



# Ray Functions and Actors

- A Ray parallel application is constructed with python decorations:

Task executed at a worker

```
@ray.remote
def simpleFunction(a, b):
    # wait for 5 seconds
    time.sleep(5)
    # return sum
    return a + b
```

Actor process

```
@ray.remote
class Counter(object):
    def __init__(self):
        self.value = 0

    def increment(self):
        self.value += 1
        return self.value
```

```
# this returns immediately
r = simpleFunction.remote(2, 4)

# this will be executed
# after 5 seconds
print( ray.get(r) )
```

Driver application