Cloud-native management of scientific workflows

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Motivation and objectives

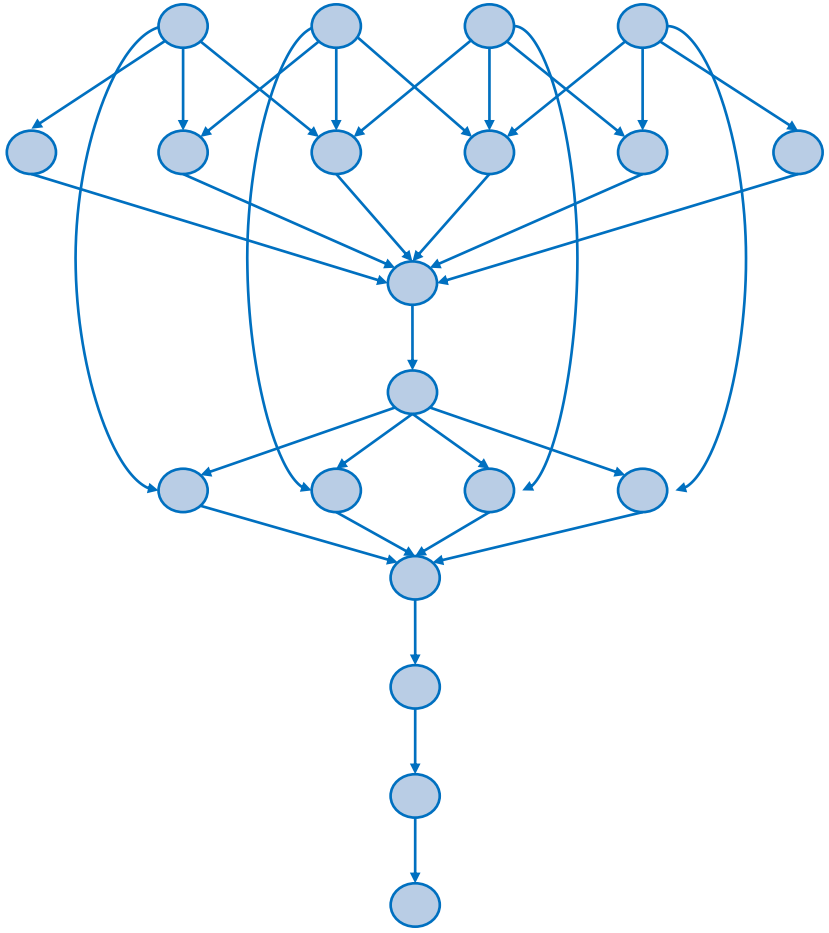
Leverage Kubernetes for scientific applications

- Resource management and scalability
- Workload scheduling
- Cloud agnostic deployment
- Rich ecosystem

Scientific workflows: large-scale graphs of tasks

- 10k-1M tasks, parallel stages, exchange data via files, use legacy software

Objective: (semi-)serverless execution with horizontal and vertical scaling using Kubernetes



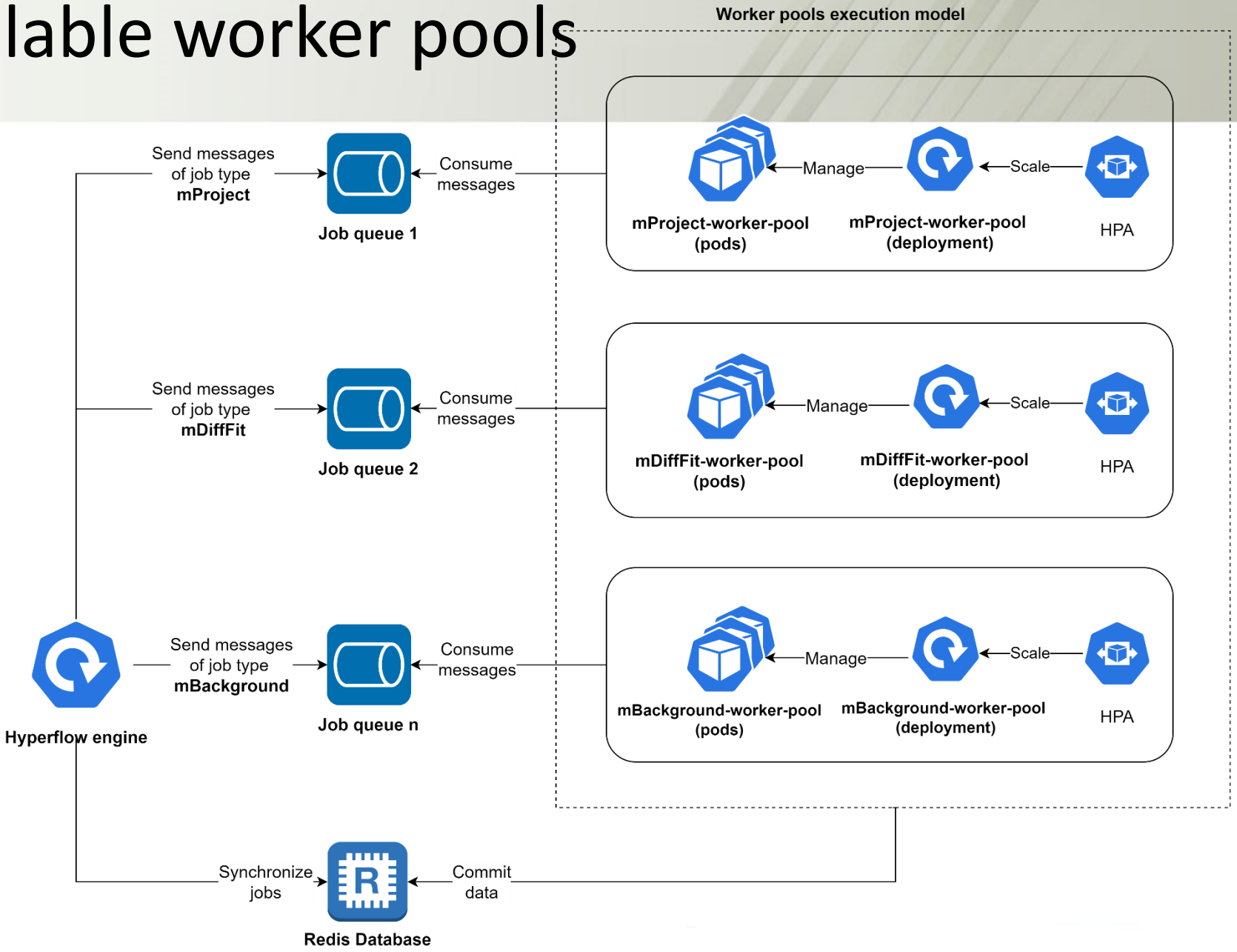
Solution: scalable worker pools

Horizontal scalability

- Proportional to queue size for that pool
- Multiple worker pools scale within an assigned resource quota

Vertical scalability

- Dynamic adjustment of CPU/Mem requests
- Using Vertical Pod Autoscaler (VPA)

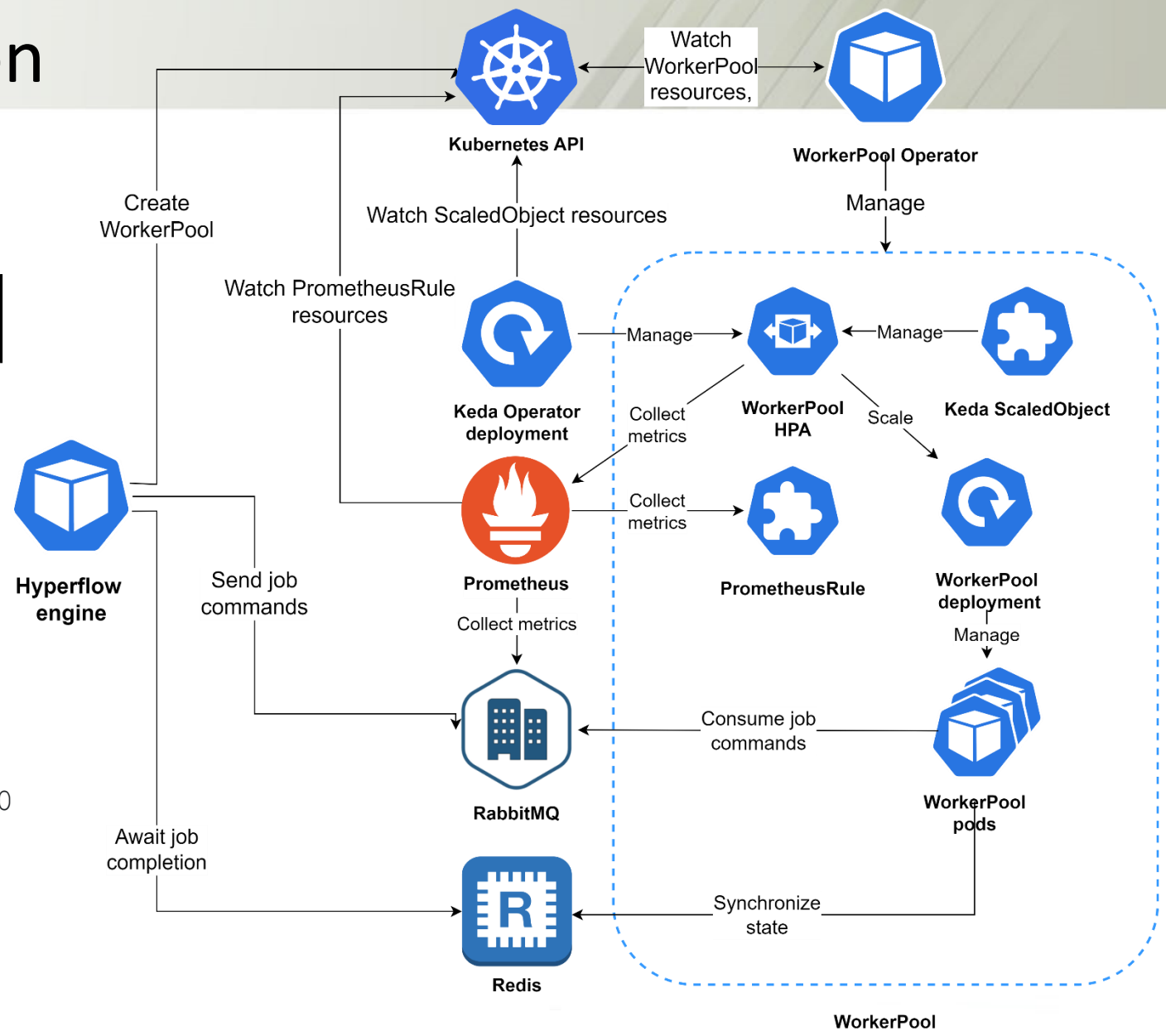


Worker pools: implementation

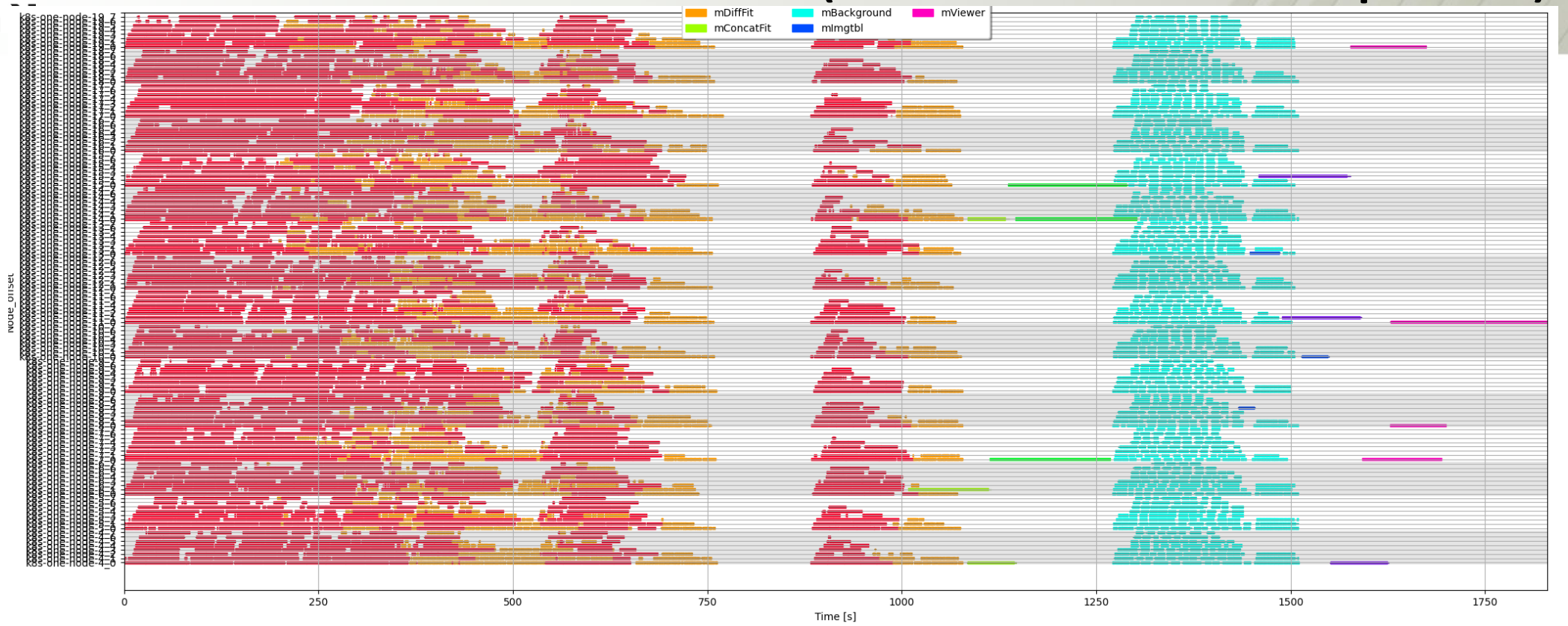
$$\boldsymbol{replicas}(\boldsymbol{w},\boldsymbol{t}) = 0.9 * \left\lceil \frac{q\_size_w\ (t)}{\sum_{\omega \in W} q\_size_\omega(t)} * \min\left(\left\lfloor \frac{cpu\_quota}{cpu\_req_w(t)} \right\rfloor, \left\lfloor \frac{mem\_quota}{mem\_req_w(t)} \right\rfloor \right) \right\rceil$$

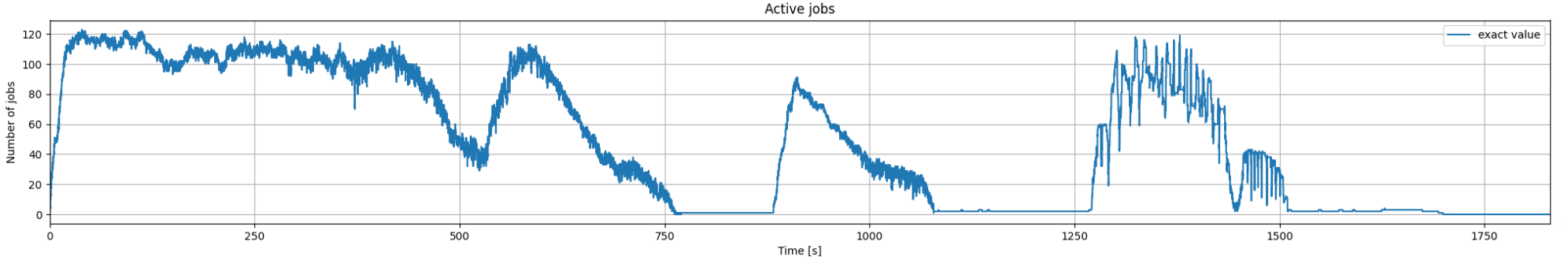
Worker Pools CRD (custom resource definition)

```yaml
apiVersion: hyperflow.agh.edu.pl/v1
kind: WorkerPool
metadata:
  name: mproject
spec:
  taskType: mProject
  image: hyperflowwms/montage2-worker
  rabbitHostname: rabbitmq.default
  prometheusUrl: http://mon-prometheus.default:9090
  redisUrl: redis://redis:6379
  minReplicaCount: 0
  maxReplicaCount: 50
  initialResources:
    requests:
      cpu: "0.5"
      memory: "524288000"
```

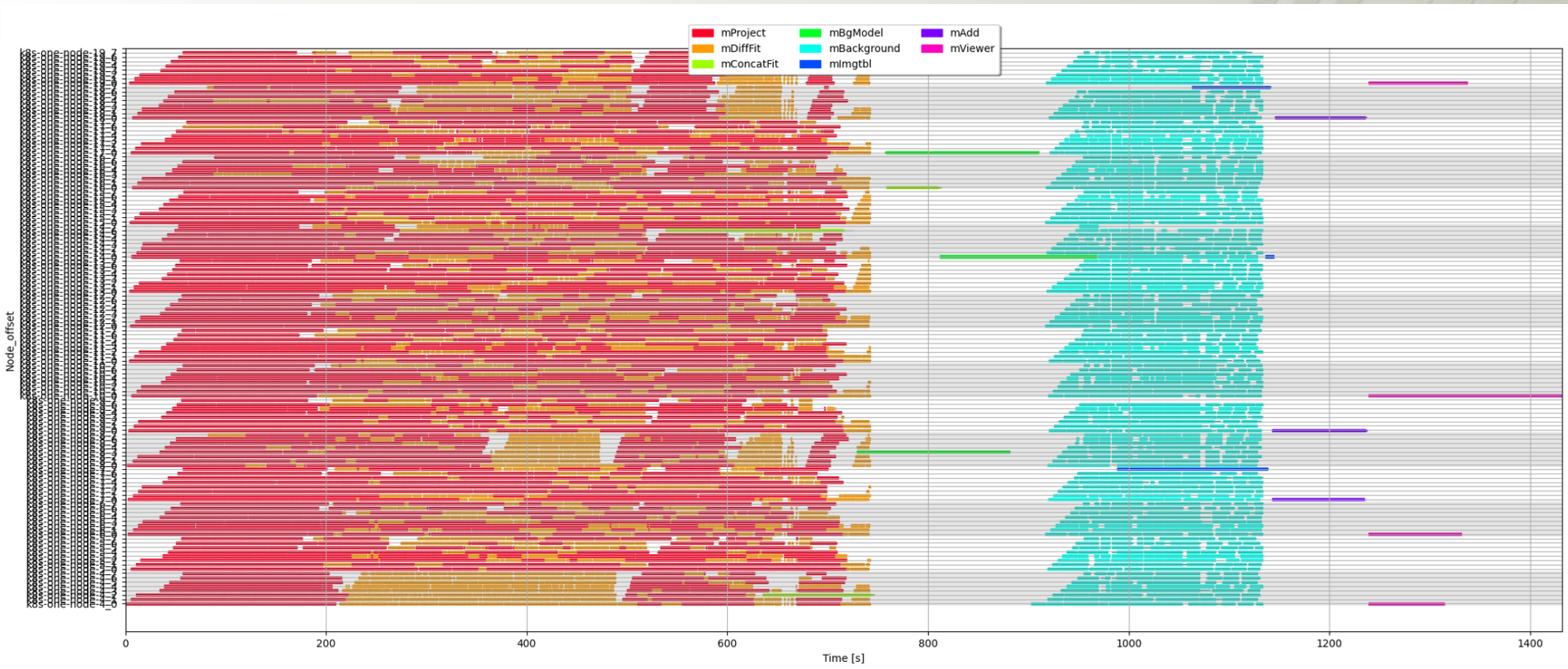


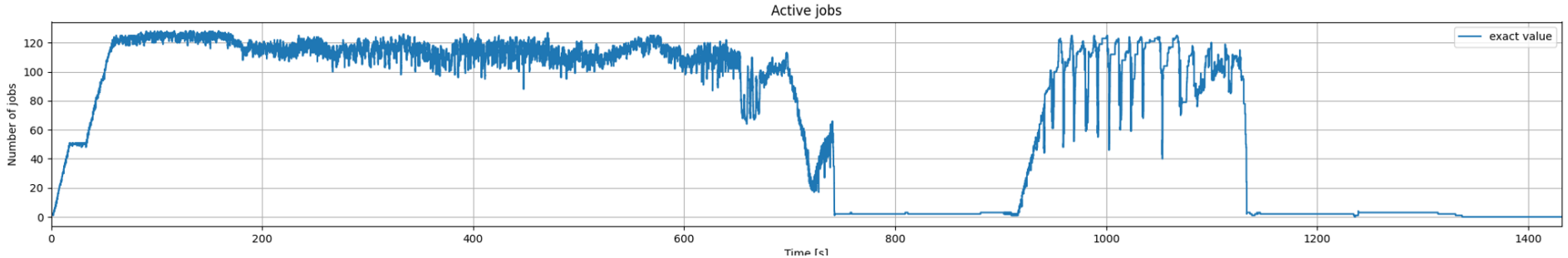
Workflow execution (without worker pools)





Montage execution: worker pools





No vertical scaling (GKE cloud)

With vertical scaling (GKE cloud)

QUESTIONS?

Institute of Computer Science AGH
http://informatyka.agh.edu.pl/en
Sano Centre for Computational Personalized Medicine
https://sano.science

HyperFlow
https://github.com/hyperflow-wms

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