Hyperparameter optimisation for Machine Learning using iDDS

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Introduction: HPO service in ATLAS

- (Needless to say the importance of hyperparameter optimisation for ML training.)
- The goal is to provide an HPO service to ATLAS users for Machine Learning
  - Minimal user code adaption
  - Support for advanced search algorithms in addition to the traditional grid or random search algorithms
  - Visualisation of results
  - To integrate geographically distributed GPU resources to provide a single resource pool to end-users
- Single-function-call pattern for HPO
  - Computing resources are managed behind the scene
  - Not suitable since ATLAS has its own resource management
- Ask-and-tell pattern for HPO
  - Decoupled optimisation+sampling from training in space-time
  - Purely point searching, no resource management
  - We go in this way

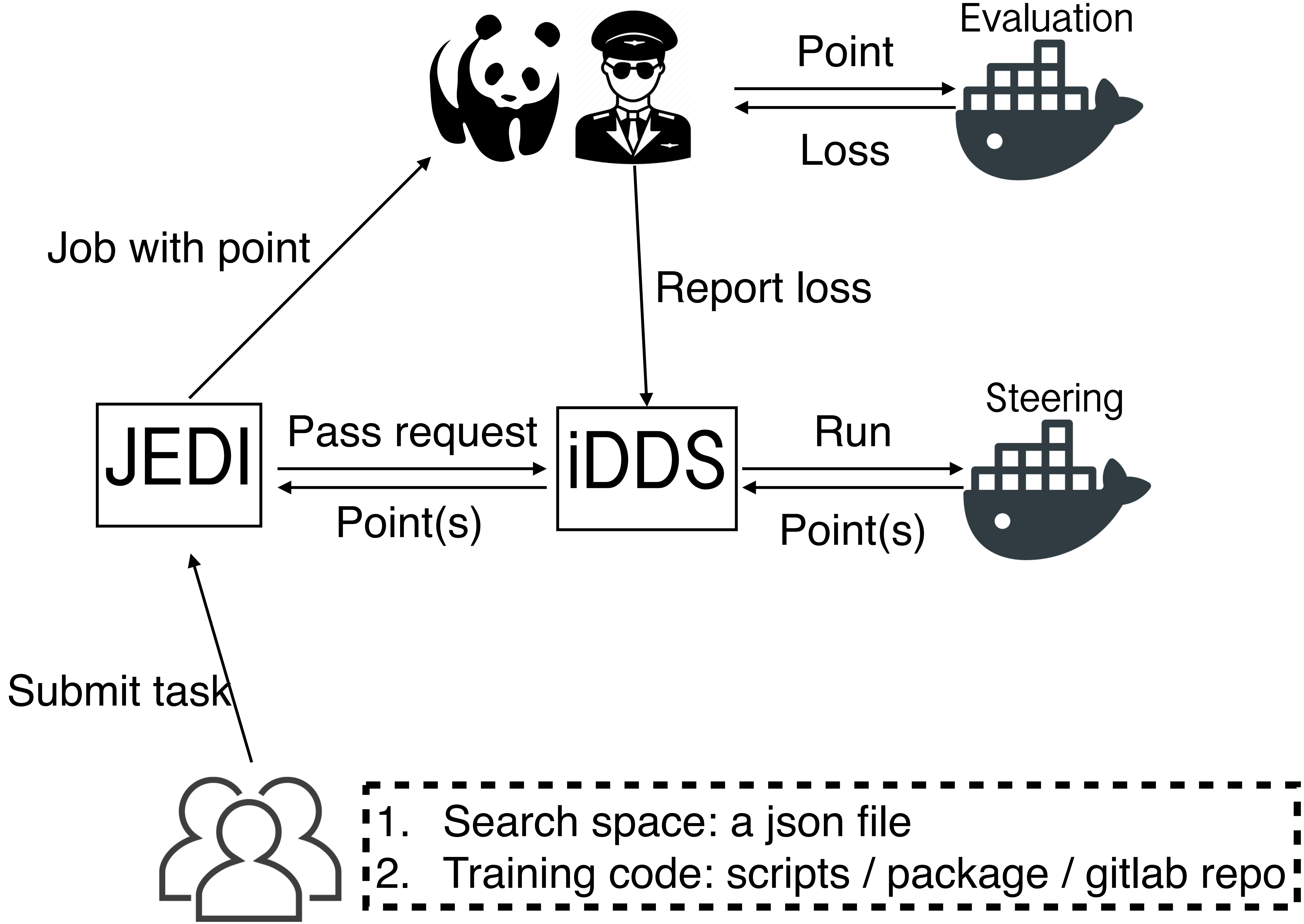
"The ask-and-tell pattern"

```
while ~ opt.stop
  x = ask(opt)
  y = f(x)
  opt = tell(opt, x, y)
end
```

The intelligent Data Delivery Service (iDDS)

- iDDS is designed to intelligently transform and deliver needed data to workflows in a fine-grained way.
  - My takeaway: jobs of successive tasks start as soon as possible, no need waiting for precedent tasks to finish, optionally making decisions in between
  - Many applications share this paradigm (documentation for currently supported use cases), e.g.:
    - Data Carousel: job starts when its input is ready, no waiting for the full dataset to be transferred
    - A chain of tasks (DOMA): successive jobs start when enough inputs are produced by the precedent tasks
    - A chain of tasks (Active Learning): successive jobs are created and submitted by iDDS based on results of precedent tasks => extendable to a generic function-as-a-service type of workflow
- HPO is a series of tasks with decision-making in between - another use case

The HPO workflow



Containerisation of the workflow

✤ Two containers to fulfil the loop:

Steering

- `SteeringContainer` - optimisation at iDDS server
  - Generate next HP points with customised method
  - A wide range of HPO methods are supported

Evaluation

- `EvaluationContainer` - ML training at Grid (GPU) sites
  - Submodule `payload` contains model definition, training scripts (user specific)

HPCs as GPU resources

- Summit as an example
  - 4608 computer nodes
    - 2 Processors x 22 cores / node
    - 6 V100 GPUs / node
  - Wonderful workstation for ML/HPO
- Challenges
  - Short wall time
  - Standard Grid services and workflows unavailable or suboptimal

HPCs as GPU resources

- Solutions
  - Checkpointing supported in the HPO workflow
  - Evaluation containers with power9 or multi-architecture support
  - Harvester on edge to mediate communication between evaluation containers and iDDS/PanDA for network-less compute nodes
  - Leveraging the data transfer service at each HPC centre not officially adopted in Rucio
  - Evolutionally specialised workload:
    1) Multiple single-GPU payloads on a single node
    2) A multi-GPU payload on a single node
    3) A multi-node/GPU payload on a static multi-node cluster
    4) A multi-node/GPU payload on a dynamic multi-node cluster for elastic distributed training

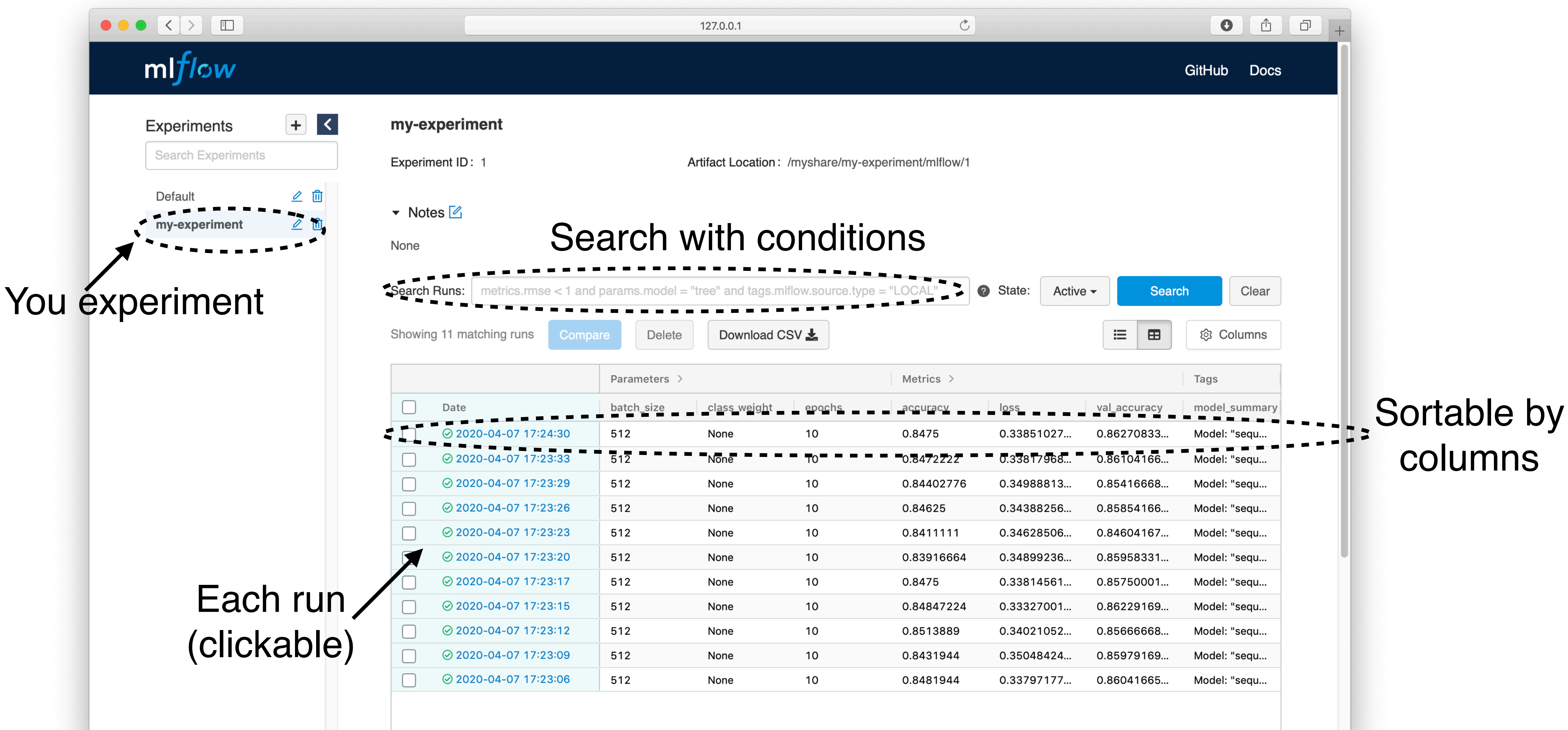
Summary

- Aim was to provide users resources for ML/HPO
  - Running with Grid site in production. Being extended to run with Google and Amazon cloud resources.
  - Running on HPC/Summit is in progress
- A survey is sent out from Physics Coordination on how much GPU resources are/will be needed by ATLAS users

Backup

Visualisation

- By default `MLflow` is turned on in `EvaluationContainer`
  - Offline visualisation on any laptop with MLflow installed is possible
  - More than visualisation - it is a ML lifecycle system
- Working with the PanDA Mon team to get a visualisation directly from Panda



Documentations

- Walk-through the Calo Image-based DNN example
  - SteeringContainer: https://gitlab.cern.ch/zhangruihpc/SteeringContainer
  - EvaluationContainer: https://gitlab.cern.ch/zhangruihpc/EvaluationContainer
- How to submit HPO task
  - https://twiki.cern.ch/twiki/bin/view/PanDA/PandaHPO
- iDDS Readme about the interfaces of ask-and-tell pattern
  - https://idds.readthedocs.io/en/latest/usecases/hyperparemeter_optimization.html