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Hyperparameter optimisation workflow using ATLAS Grid

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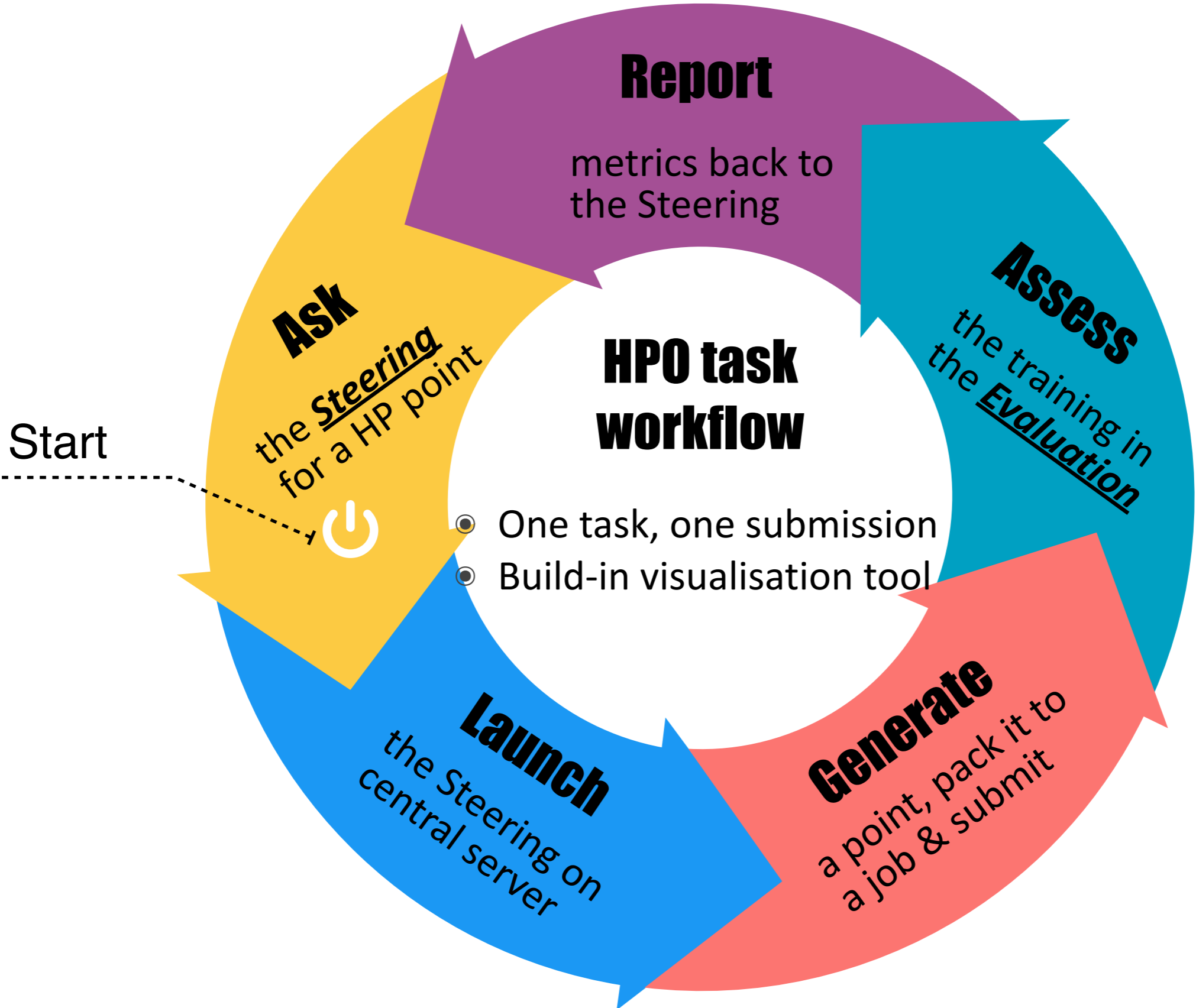
HPO service in ATLAS

- ❖ Hyperparameter optimisation (HPO) is a resource-intensive task
 - Usually need to run through full training for each possible HP set
- ❖ Our goal is to provide an HPO service to ATLAS users on Grid
 - Minimal user code adaption
 - Wide support for optimisation algorithms
 - Visualisation of results
- ❖ 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

“The ask-and-tell pattern”

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

The workflow



Steering container

- Run on central servers
- One container for all users
- Rich optimization algorithms
- Unified search space format

Evaluation container

- Run on Grid sites
- Encapsulate training job
- User customizable
- Accessible to data on Grid

Report

metrics back to the Steering

Ask

the Steering for a HP point



HPO task workflow

- One task, one submission
- Build-in visualisation tool

Assess

the training in the Evaluation

checkpointing

- In case of short walltime on sites
- Periodically upload checkpoints to Grid
- Download the checkpoint when retrying
- Resume training if checkpoint is found

Summary

- ❖ A central computing service is built up for ATLAS users to run hyperparameter optimisation
 - Utilise ATLAS PanDA system as base infrastructure
- ❖ Rich optimisation libraries are supported
 - hyperopt, skopt
 - Nevergrad
- ❖ One HPO task, one submission
 - Grid component to bookkeeping search points in use defined search space
- ❖ Containerised workflow
 - Training jobs in container - fully customisable, fully preservable