ML Service with PanDA and iDDS

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NPPS/Omega/EDG joint meeting on AI/ML in BNL Physics 16 April 2021

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Introduction

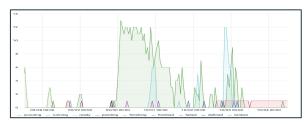
- The goal of the ML service project is to provide a service to users for ML-related activities with PanDA and iDDS
 - Scalability and resource integration through PanDA ecosystem
 - Leveraging new capabilities brought by iDDS
 - Decoupling of data delivery and execution
 - Description of workflow with directed acyclic graph (DAG)
 - Orchestration of workflow management system and data management system
 - Modern user auth and interface
- > Functions
 - Hyperparameter optimization
 - Parallel training of multiple ML models
 - Elastic distributed training
 - Feedback loops to refine new iterations based on the results of old iterations
 - Task graph for advanced workflows
 - Visualization

Intelligent Data Delivery Service (iDDS)

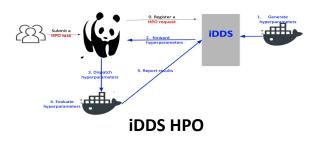
- > Joint ATLAS and IRIS-HEP project launched in 2019
- Designed to intelligently deliver needed data and workload in a fine-grained way
- > Usecases
 - Data Carousel
 - Jobs start when its own input is ready, no wait for the full dataset to be transferred
 - In production in ATLAS since May 2020
 - Solved the issues with the delayed start of data processing on tape
 - HPO (Hyper Parameter Optimization)
 - To provide a fully-automated platform for hyperparameter optimization on top of geographically distributed GPU resources on the grid, HPC, and clouds
 - Advertised to ATLAS ML users, not specific to ATLAS
 - DAG-based workflow management
 - High-level workflows specified by DAGs driving workload scheduling where successive jobs start off once all dependent jobs are done
 - Cascade of chains for multi-step processing with thousands of jobs per step
 - Release jobs incrementally for different steps to avoid long waiting time
 - Using DOMA PanDA and iDDS instances for Rubin Observatory (LSST) exercise

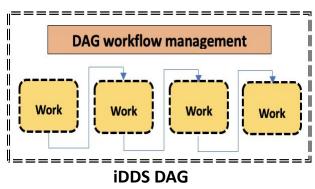


(Wen Guan)



iDDS tasks accounting (by status)





Hyperparameter Optimization Service

Hyperparameter Optimization (HPO)

- > The problem of choosing a set of optimal hyperparameters for a ML model
 - A hyperparameter = A parameter whose value is used to control the learning process
 - Parameter scan in a search space \rightarrow a whole training session for each parameter point \rightarrow computationally intensive
- > Usage of GPU resources is crucial
 - Well optimal for linear algebra operations that play a key-role in ML training
 - PanDA's capability to easily integrate heterogeneous resources

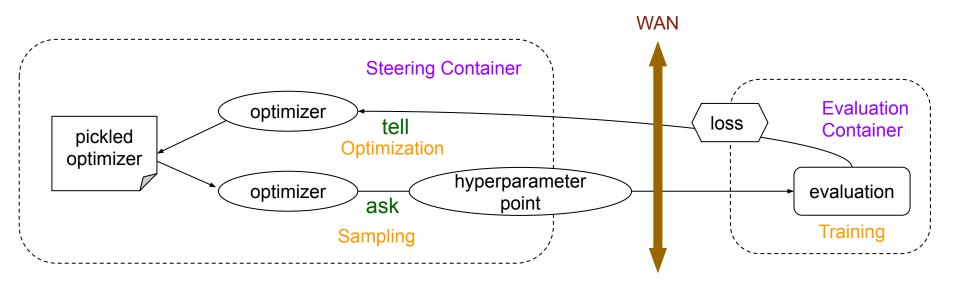
> HPO in existing ML packages

- Single-function-call pattern
 - A kind of a blackbox that manages computing resources behind the scene
 - Not suitable to work with PanDA since PanDA has its own resource management mechanism
- Ask-and-tell pattern
 - Asynchronous execution of sampling, training, and optimization steps
 - Purely point searching, no resource management

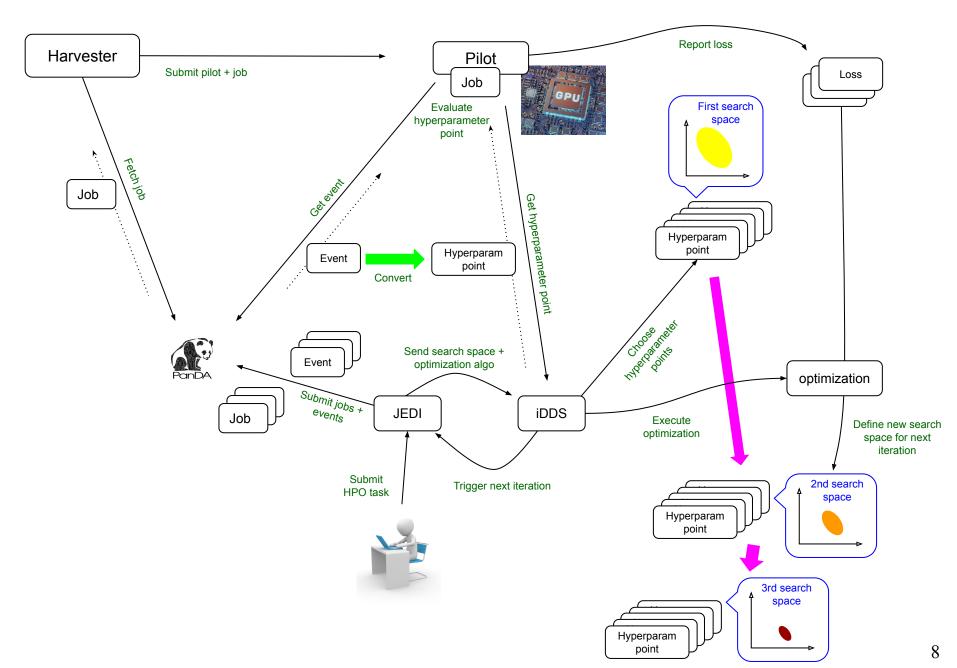
```
"The ask-and-tell pattern"
while ~ opt.stop
  x = ask(opt)
  y = f(x)
  opt = tell(opt, x, y)
end
```

Ingredients of HPO Workflow

- \succ Two types of containers
 - Steering container optimisation on central iDDS server
 - Generate next HP points with customised method
 - A wide range of optimization algorithms are supported
 - Evaluation container training at remote grid (GPU) sites
 - Submodule payload contains a ML model definition and user-specific training
- > Checkpointing
 - Periodically upload checkpoints to Grid
 - Download the checkpoint when the same job is retrying
 - Resume training if checkpoint is found

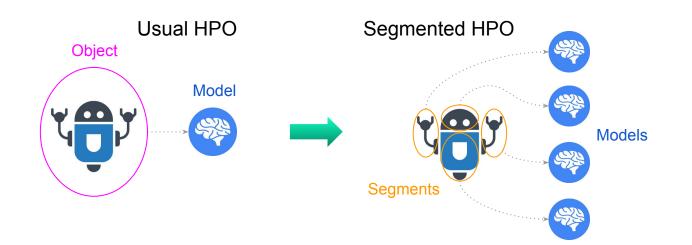


HPO Service with PanDA and iDDS

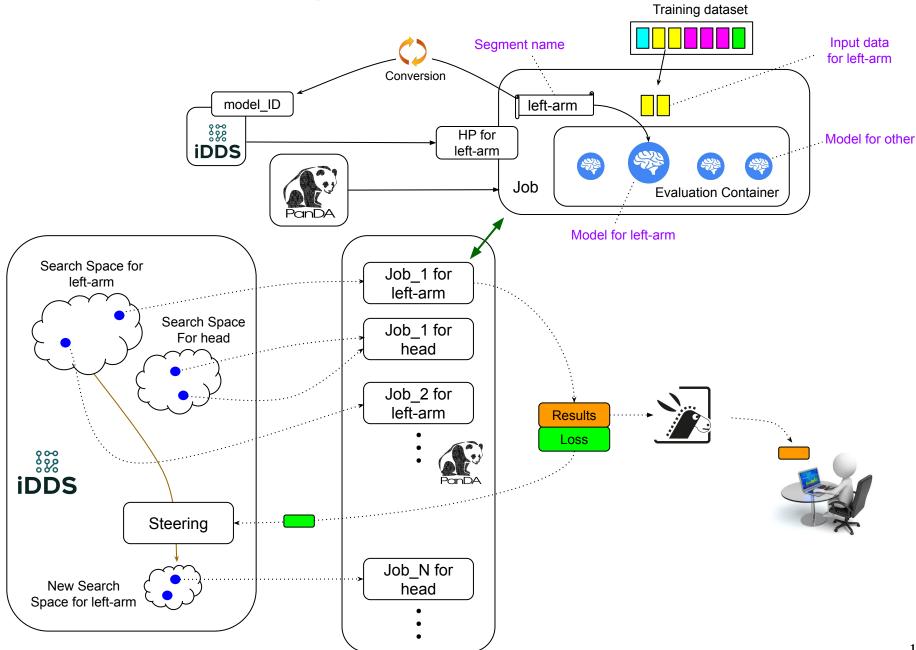


Segmented HPO

- > Some ML payloads can be logically broken down
 - E.g. break-down of a single physics search session into multiple search sessions targeting different physics regions/entities
- > A real ATLAS example: FastCaloGAN, a calorimeter image generation model
 - 300 GANs = 300 models = 100 η slices x 3 PIDs
 - 100 GPU-days to train 300 GANs
 - 300 individual tasks in the usual workflow \rightarrow Bookkeeping nightmare
- > Segmented HPO
 - A single HPO task to optimize all ML models in one-go
 - Concurrent training of multiple models, and a smaller training dataset for each model
 - Fast turnaround
 - Execution of workloads on more distributed resources



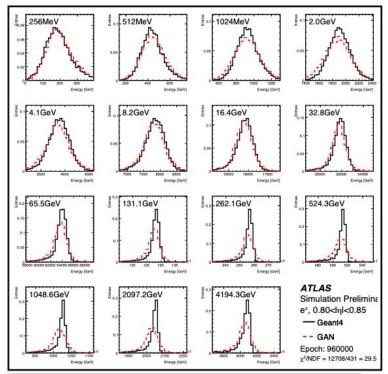
Segmented HPO Workflow



Test Results with FastCaloGAN

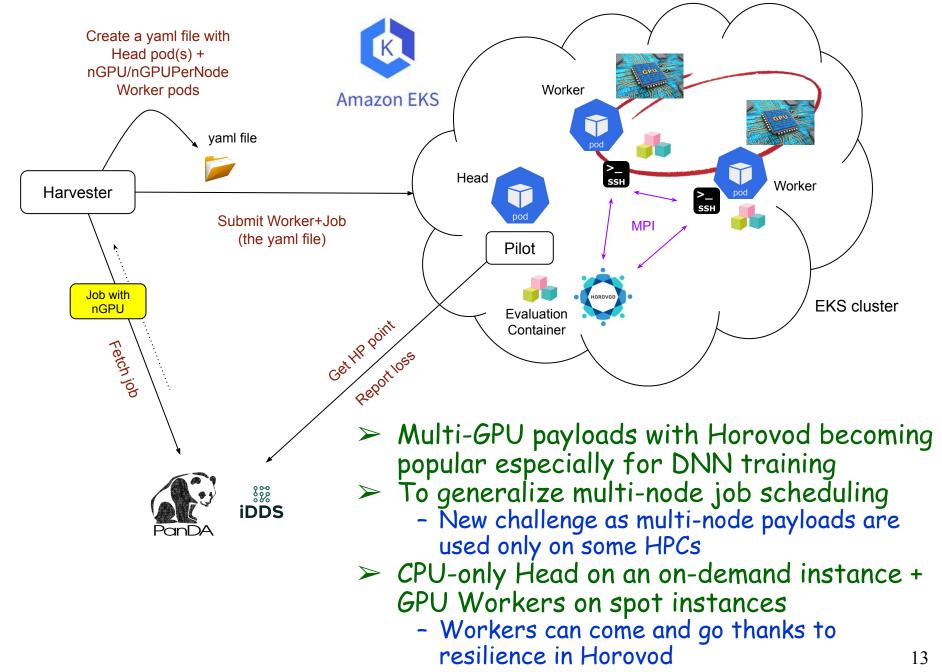
- \succ Tested with 15 GANs (15 segments)
 - 3 particle types × 5 η slices
 - Grid search as still needs offline analysis of training results
- Staged only relevant data for each GAN rather than sending the whole data in the training dataset
 - Minimized data motion
- Reasonable results shown in the plots on the right from a 10K-epoch job running on the BNL GPU site
- Foreseen full automation with more advanced search algorithm once the procedure of the offline analysis is well established

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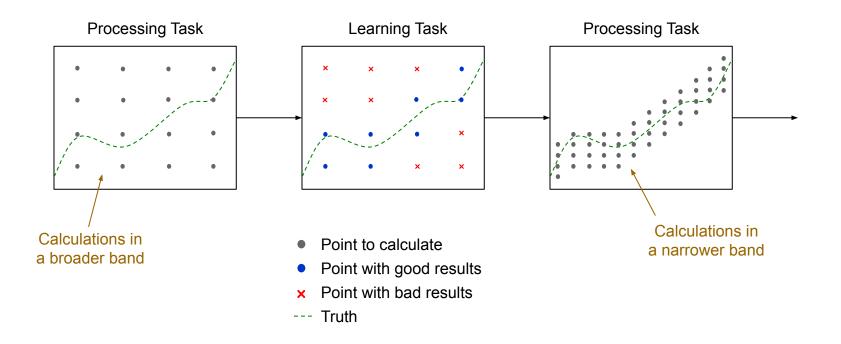
Ongoing Development Activities

Distributed Training with Horovod on Amazon



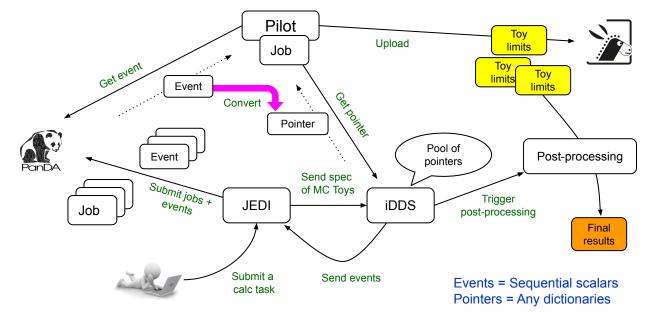
Active Learning

- > To define the subsequent processing task based on the decision making in the learning task which analyzes the results of the previous processing task
 - Task chain + decision making between
 - A simple DAG usecase
- Two types of task templates to generate concrete tasks, and condition branches to control the workflow
- \succ Being integrated in the system



RootStats-based Limit Calculation with MC Toys

- > 10000 MC toys would take approximately 55 hours to run, according to Xola's slides \rightarrow Offloading random number generation to GPU
- > Materials in Christian's repo: https://gitlab.cern.ch/chweber/StandardHypoTestInv
- > Mapping to the system as a chain from toy limit calculations to post-processing without iteration
 - iDDS has a pool of pointers to MC toys
 - Each job takes a pointer to calculate the relevant toy limits and takes another pointer if the walltime is still available
 - iDDS triggers the post-processing that combines toy limits to the final results



Visualization Support for HPO

- > A visualisation tool MLflow is turned on in Evaluation Container
 - Useful for offline visualisation and analysis
- > An α -version of the tool also integrated into PanDA Monitoring system
 - Fetch output from training jobs and centrally spin-up an MLFlow container to display results
 - Extendable to other visualisation tools (Neptune, WandB, Tensorboard, etc.)

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User Interface in Jupyter Lab

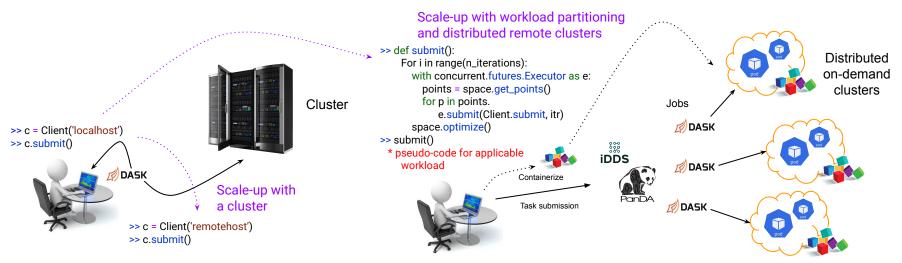
- > Jupyter Notebook has become a popular user interface for research science, data science, data analytics, and ML
- > Access to PanDA/iDDS from Jupyter
 - Seamless integration with user's analysis environment
 - Remote resources through PanDA/iDDS
- Easy to provide sophisticated look-and-feel especially for advanced workflows
 - E.g., a visual interface to define and control task networks for DAG workflows
- > Thousands of extensions/tools in Jupyter ecosystem

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Running Dask through PanDA/iDDS

- > Dask is a Python library for parallel computing
 - Very easy to parallelize your analysis written with other Python projects such as NumPy, pandas, scikit-learn, etc
 - Built-in capability for seamless scale-up with clusters
- > To offer further scale-up with workload partitioning and distributed remote clusters
 - Depending on characteristics and requirements of each workload
 - E.g. distributed training with Dask instead of Horovod
- Another type of multi-node payloads from the system point of view
 - Trying to reuse the mechanism that has been originally developed for Horovod payloads
- > GCP as a part of Google R&D Y2, EKS, other k8s-based resources



Conclusions

- > PanDA/iDDS-based HPO service is up and running
 - Experiment agnostic implementation
 - Support of both usual and segmented HPO workflows
 - Available for ATLAS users on ATLAS instances and for other experiment users on DOMA instances
- Many ongoing development activities to add ML-related functions to the service
 - HPO service \rightarrow ML service
- > Usecase-driven project
 - Inputs/feedbacks from (BNL) physics communities are highly appreciated
 - E.g., came up with the idea of RootStats-based limit calculation in a meeting with Christian
 - Happy to support more usecases
 - HPO Documentation:

https://panda-wms.readthedocs.io/en/latest/client/phpo.html