

TRAINING & OPTIMISATION OF LARGE TRANSFORMERS

ATLAS CASE STUDY ON KUBEFLOW

JET FLAVOUR TAGGING

CLASSIFICATION TASK

Labels

b, c, light, τ

Inputs

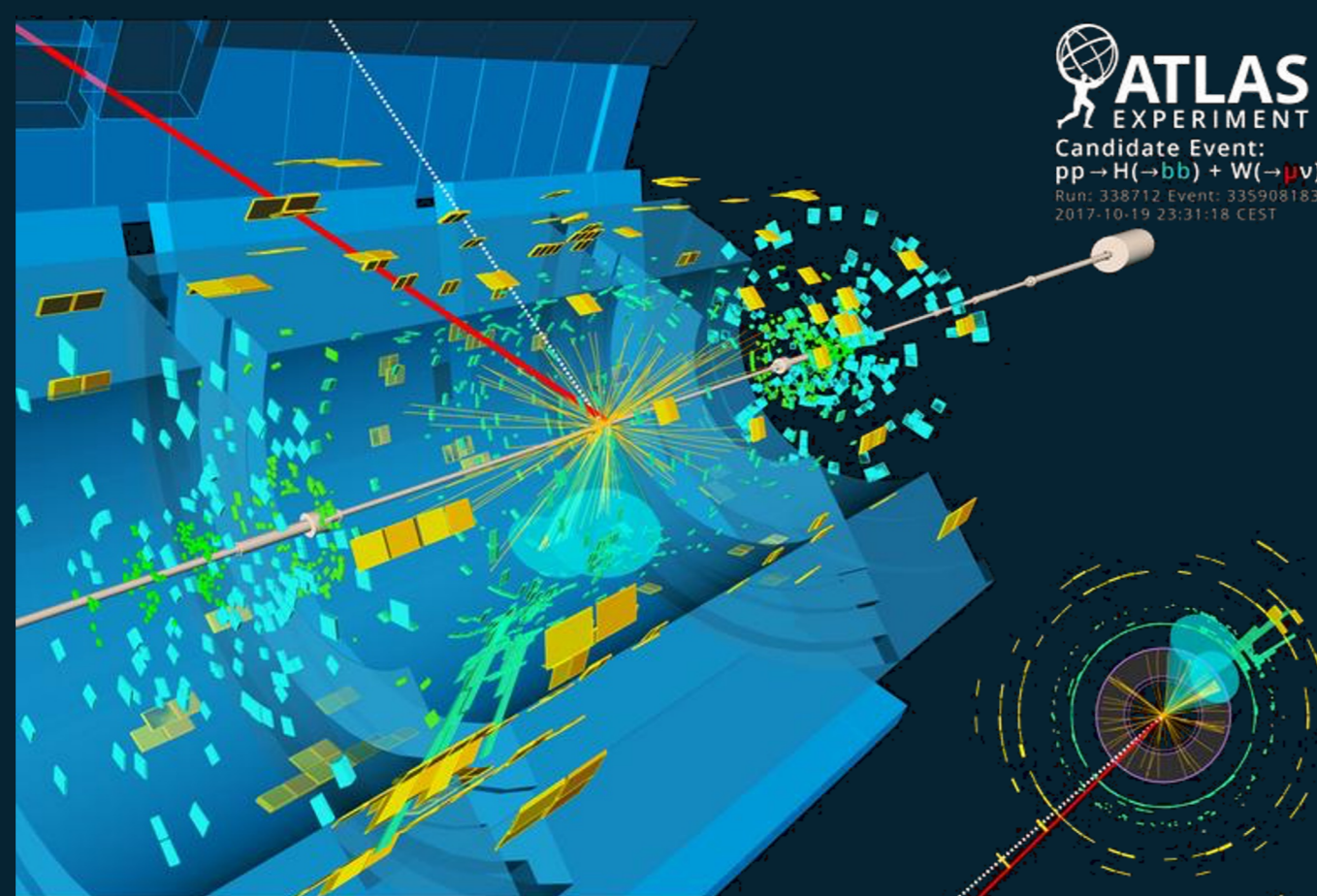
Tracks + jet information

Outputs

Per-flavour probability + Discriminant

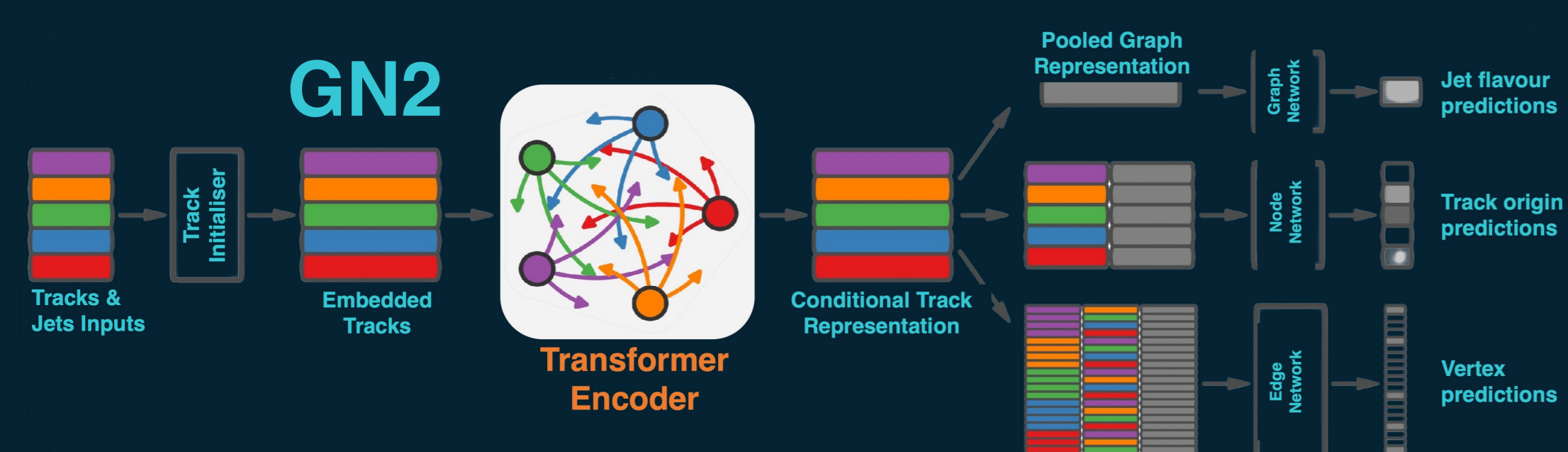
Used in ATLAS:

$H \rightarrow b\bar{b} | c\bar{c}$, di-Higgs, ...



ATLAS event display of a Higgs boson decaying to two b-quarks

SOTA: Multimodal Multitask Transformer Model

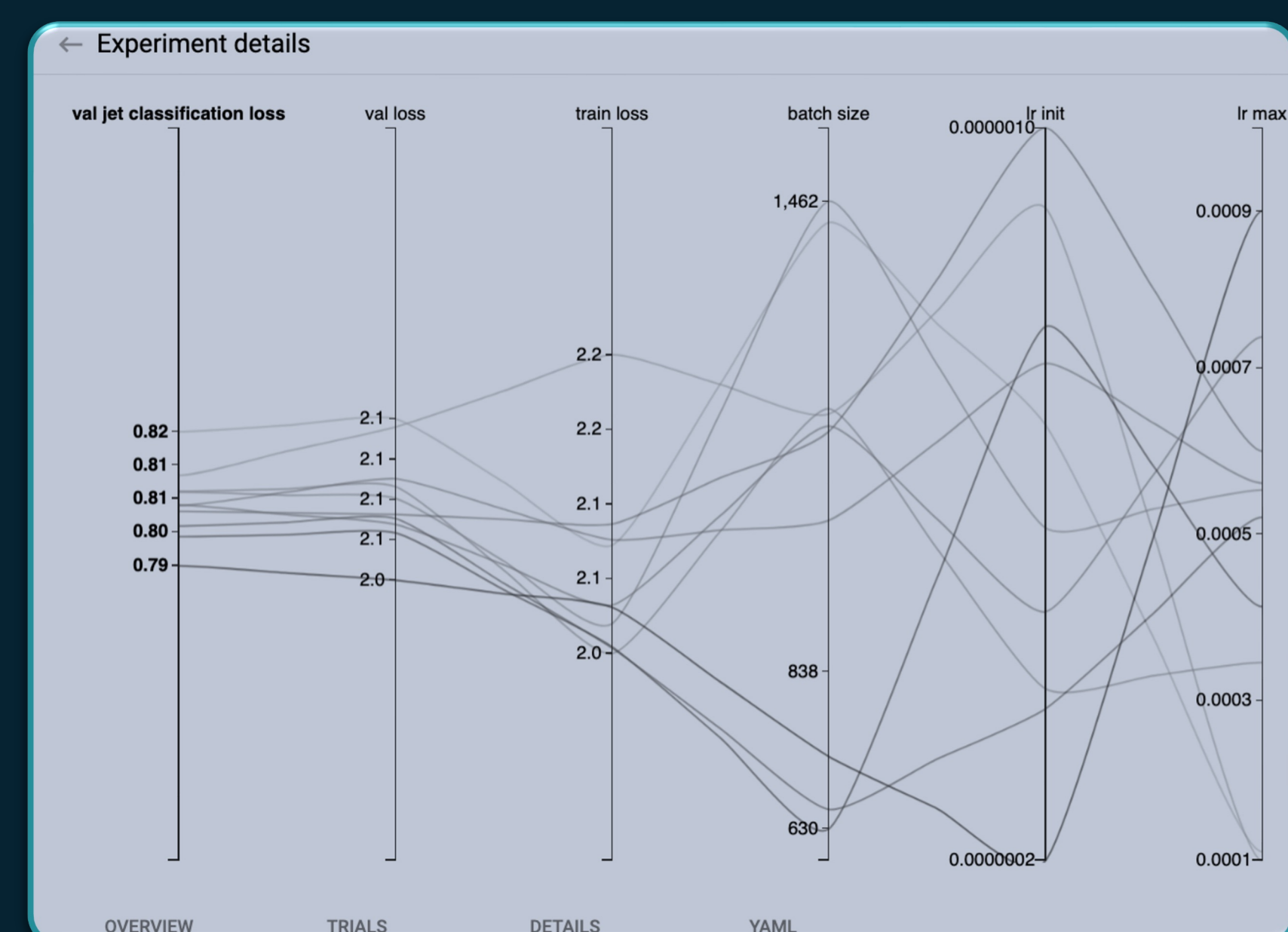
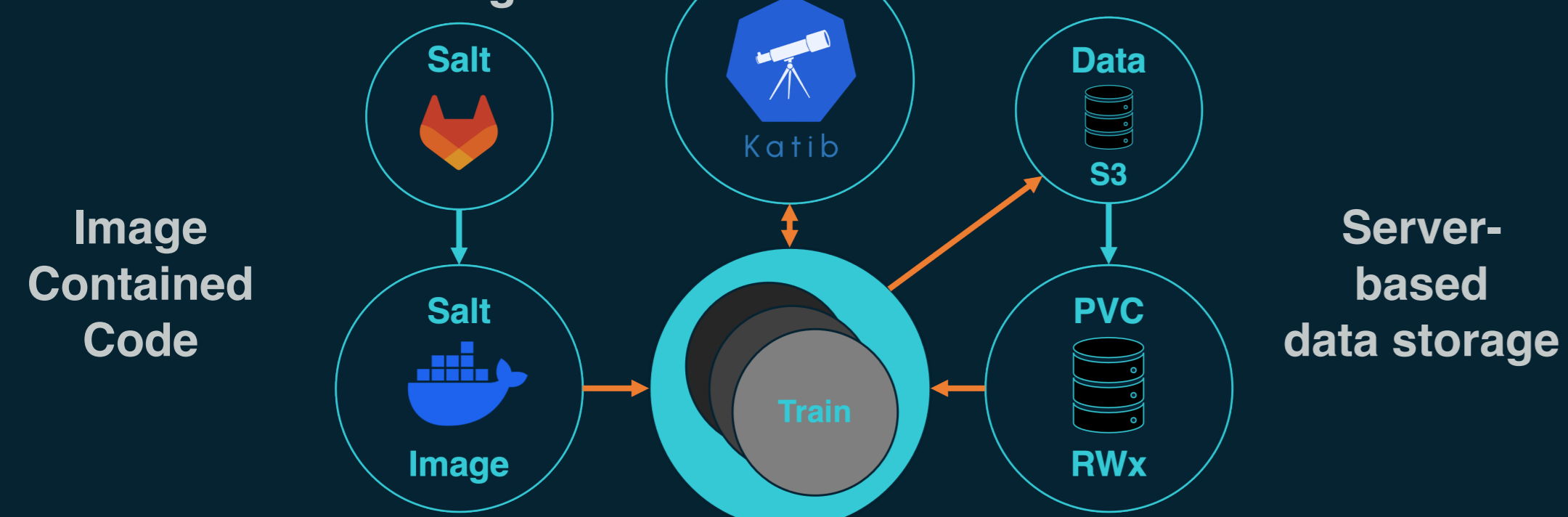


Goal Hyperparameter Optimisation (HPO)



Built on Kubernetes
Open-source container orchestration engine

Designed for MLOps
Training, Inference,
Katib HPO + AutoML



EFFICIENT DESIGN

- Multi-platform
- Resource Usage
- Monitoring
- AutoML Algorithms

PARAMETRIZATION MATTERS!

Standard Parametrization (SP)



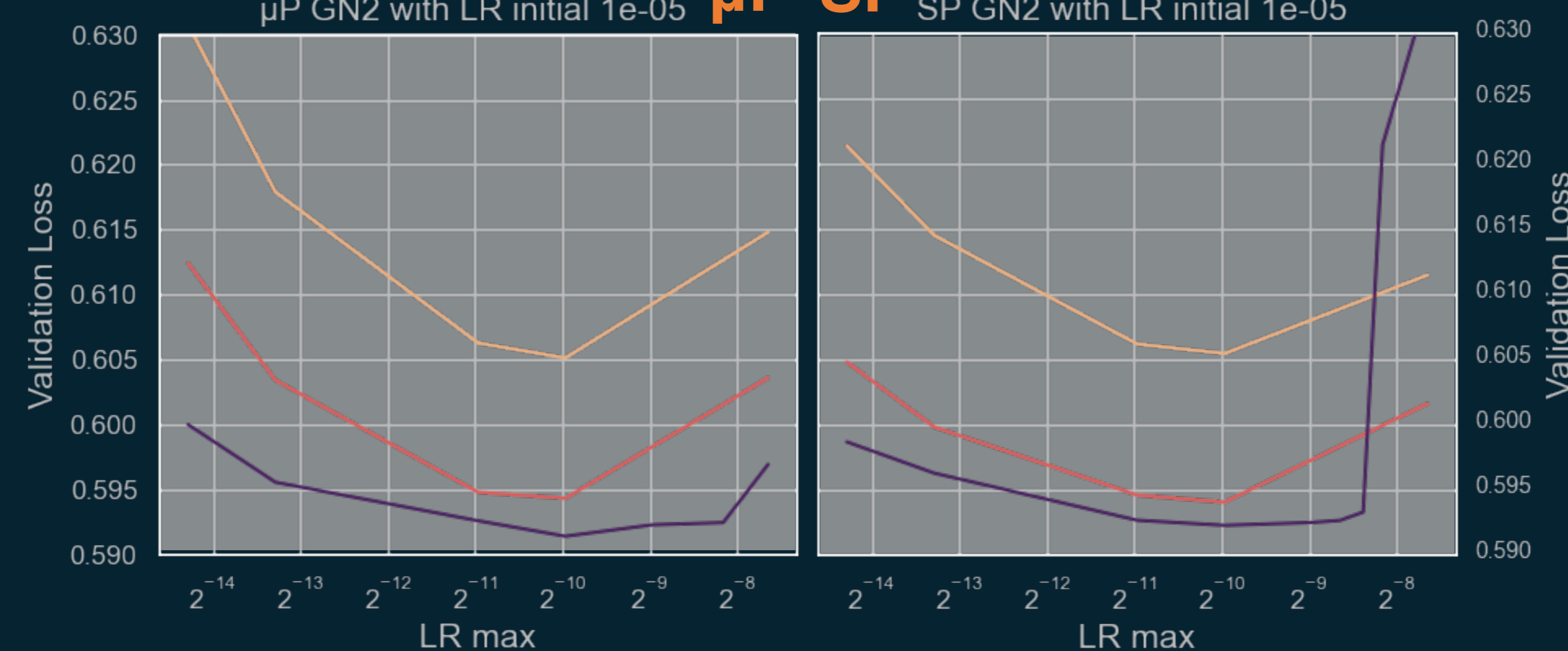
Initialisation: $W^{L_{in}} \sim \mathcal{N}\left(0, \frac{1}{d_{L_{in}}^{in}}\right)$, $W^{L_{hid}} \sim \mathcal{N}\left(0, \frac{1}{d_{L_{hid}}^{in}}\right)$, $W^{L_{out}} \sim \mathcal{N}\left(0, \frac{1}{d_{L_{out}}^{in}}\right)$, $b^{L_{...}} = 0$
 SGD & Adam LR: \forall weights η

Maximal Update Parametrization (μP)



Initialisation: $W^{L_{in}} \sim \mathcal{N}\left(0, \frac{1}{d_{L_{in}}^{in}}\right)$, $W^{L_{hid}} \sim \mathcal{N}\left(0, \frac{1}{d_{L_{hid}}^{in}}\right)$, $W^{L_{out}} \sim \mathcal{N}\left(0, \frac{1}{d_{L_{out}}^{in} \times d_{L_{out}}^{in}}\right)$, $b^{L_{...}} = 0$
 SGD LR: $\eta_{W^{L_{in}}} = \eta_{b^{L_{...}}} = \eta \times d_{L_{in}}^{out} | L_{...}$, $\eta_{W^{L_{hid}}} = \eta$, $\eta_{W^{L_{out}}} = \eta / d_{L_{out}}^{in}$
 Adam LR: $\eta_{W^{L_{in}}} = \eta_{b^{L_{...}}} = \eta$, $\eta_{W^{L_{hid}}} = \eta / d_{L_{hid}}^{in}$, $\eta_{W^{L_{out}}} = \eta / d_{L_{out}}^{in}$

ATLAS Simulation Preliminary μP GN2 with LR initial 1e-05 vs ATLAS Simulation Preliminary SP GN2 with LR initial 1e-05

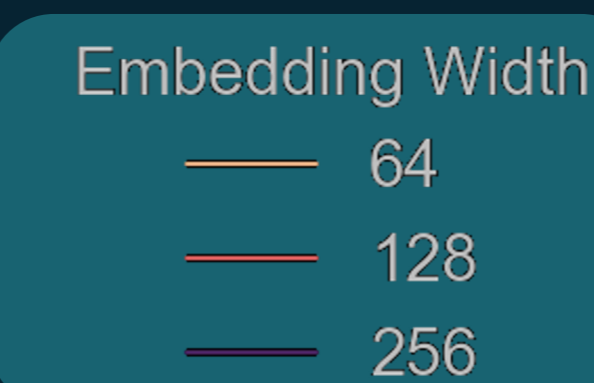


Stable for μP , blows up for SP!

μP Transfer Algorithm

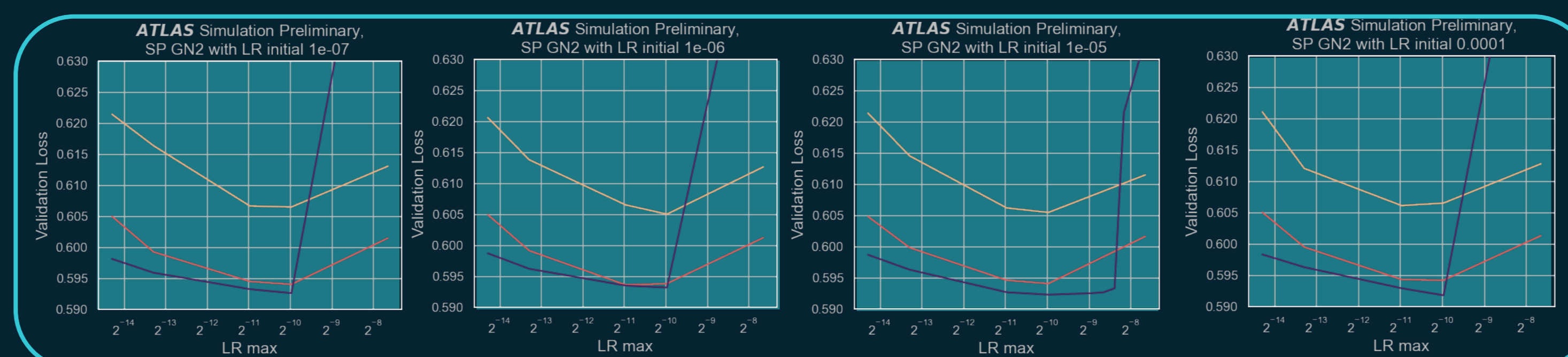


- Similar performance hierarchy between small and large models in μP
- Hyperparameter optimisation on a smaller model
- Zero-shot transfer: best low-complexity = best high-complexity model
- Wider is always better

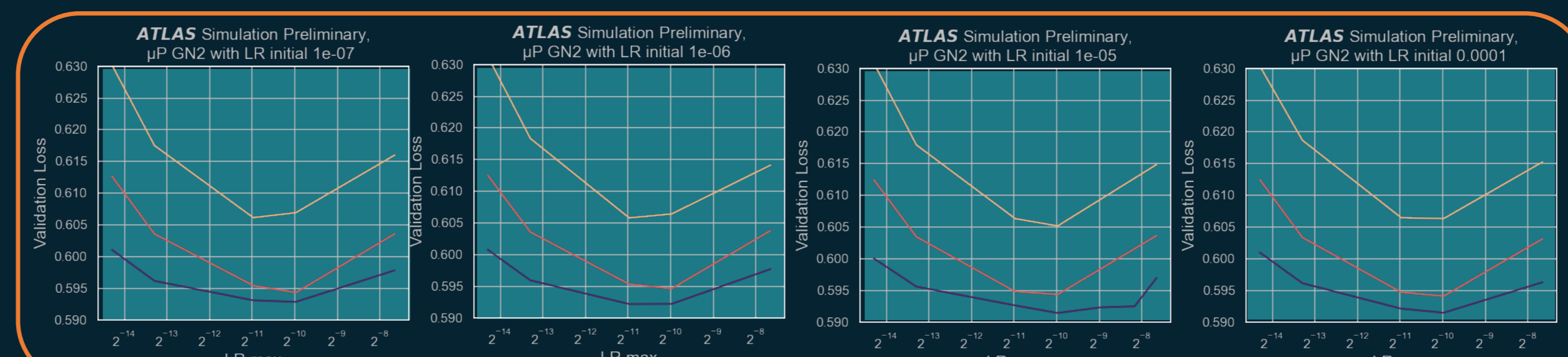


Real Deployment: LR Scheduler Optimisation (initialisation & maximal values)

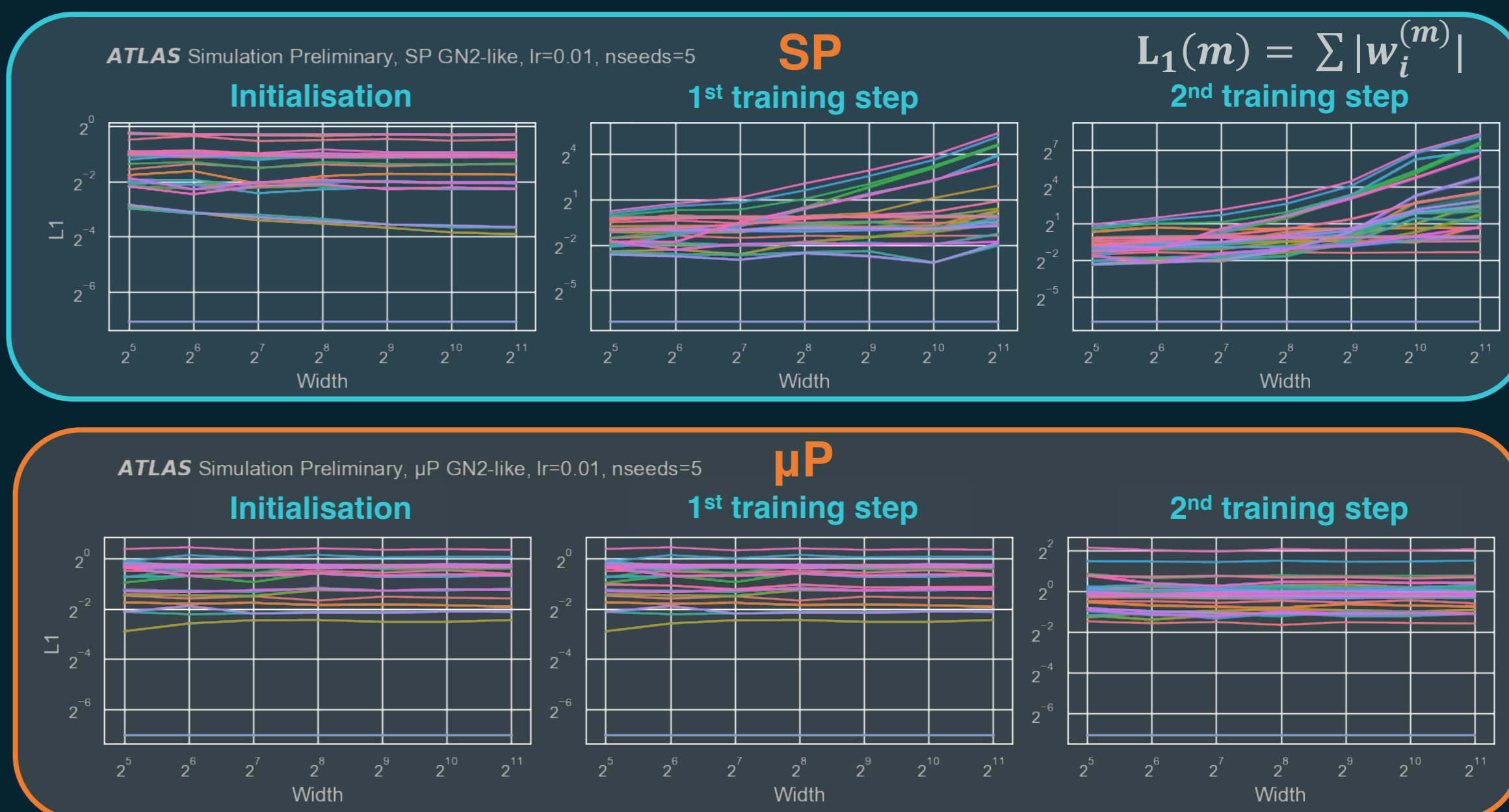
SP



μP



VERIFICATION A look at pre-activation weights



ADVANTAGES



- Multi-platform & flexible
- Hardware agnostic MLOps & optimised resource usage
- Advanced AutoML algorithms for improved HPO
- Powerful visualisation
- CERN-wide access

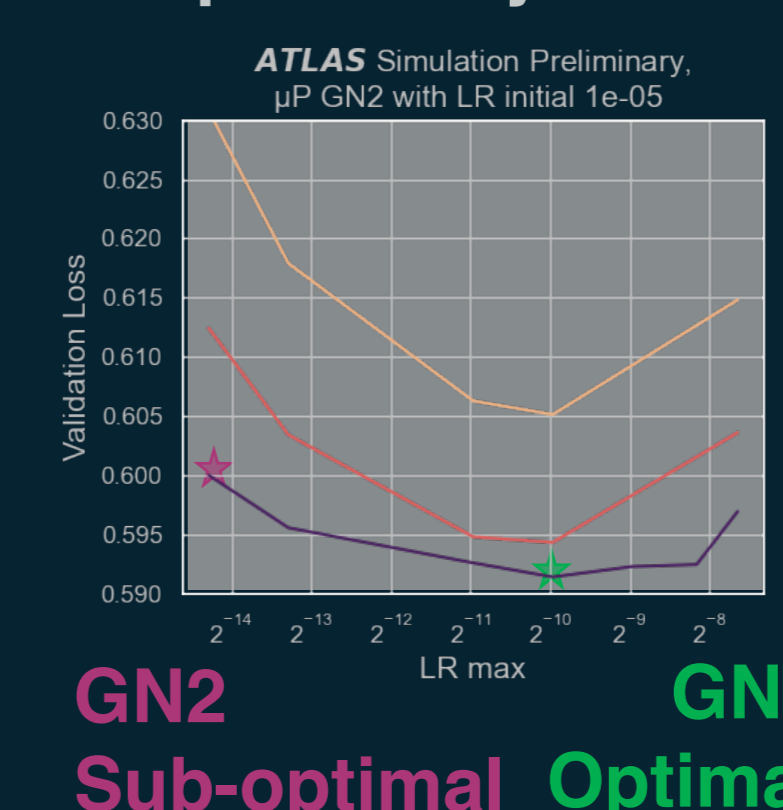
Maximal Update Parametrization (μP)

- Wider is always better \rightarrow simple neural architecture search
- μP Transfer HP zero-shot small \rightarrow large models
- Reduced computing requirement per HP set test
 - Width 256 (2.30 M params): 2 GPUs \rightarrow 39 min / epoch
 - Width 64 (0.29 M params): 1 GPU \rightarrow 20 min / epoch
- Better coverage of the HP search space
 - With μP , 4 small-model tests \approx 1 full-model test

COMBINE

HPO MATTERS

Significant performance dependency on HP



$$D_b = \frac{p_b}{f_c p_c + (1 - f_c) p_{light}}$$

