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interTwin - an Interdisciplinary Digital Twin Engine for Science

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The interTwin project, funded by the European Commission, is at the forefront of leveraging 'Digital Twins' across various scientific domains, with a particular emphasis on physics and earth observation. Two of the most advanced use-cases of interTwin are event generation for particle detector simulation at CERN as well as the climate-based Environmental Modelling and Prediction Platform (EMP2) jointly developed at CERN and the Julich Supercomputing Center (JSC) using foundation models. interTwin enables those use-cases to leverage AI methodologies on cloud to high-performance computing (HPC) resources by using itwinai - the AI workflow and method lifecycle module of interTwin.

The itwinai module is developed collaboratively by CERN and JSC and is a pivotal contribution within the interTwin project. Its role is advancing interdisciplinary scientific research through the synthesis of learning and computing paradigms. This framework stands as a testament to the commitment of the interTwin project towards co-designing and implementing an interdisciplinary Digital Twin Engine. Its main functionalities and contributions are:

Distributed Training: itwinai offers a streamlined approach to distributing existing code across multiple GPUs and nodes, automating the training workflow. Leveraging industry-standard backends, including PyTorch Distributed Data Parallel (DDP), TensorFlow distributed strategies, and Horovod, it provides researchers with a robust foundation for efficient and scalable distributed training. The successful deployment and testing of itwinai on JSC's HDFML cluster underscore its practical applicability in real-world scenarios.

Hyperparameter Optimization: One of the core functionalities of itwinai is its hyperparameter optimization, which plays a crucial role in enhancing model accuracy. By intelligently exploring hyperparameter spaces, itwinai eliminates the need for manual parameter tuning. The functionality, empowered by RayTune, contributes significantly to the development of more robust and accurate scientific models.

Model Registry: A key aspect of itwinai is its provision of a robust model registry. This feature allows researchers to log and store models along with associated performance metrics, thereby enabling comprehensive analyses in a convenient manner. The backend, leveraging MLFlow, ensures seamless model management, enhancing collaboration and reproducibility.

In line with the theme of the 2024 ACAT workshop, "Foundation Models for Physics," interTwin and its use-cases empowered by itwinai are positioned at the convergence of computation and physics and showcase the significant potential of foundation models, supported by HPC resources. Together, they contribute to a narrative of interconnected scientific frontiers, where the integration of digital twins, AI frameworks, and foundation models broadens possibilities for exploration and discovery through itwinai's user-friendly interface and powerful functionalities.

Significance

The frameworks developed within interTwin enable the integration of foundation models for physics and earth observation within a Digital Twin Engine and alleviate their development by a seamless use of advanced AI workflows powered by HPC resources.

References

Experiment context, if any

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