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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. One of the most advanced use-cases of interTwin is event generation for particle detector simulation at CERN. interTwin enables particle detector simulations 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, a comprehensive solution for AI workflow and method lifecycle developed collaboratively by CERN and the Julich Supercomputing Center (JSC), serves as the cornerstone for researchers, data scientists, and software engineers engaged in developing, training, and maintaining AI-based methods for scientific applications, such as the particle event generation. 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 first European AI for Fundamental Physics Conference of connecting AI activities across various branches of fundamental physics, interTwin and its use-cases empowered by itwinai are positioned at the intersection of AI, computation and fundamental physics. itwinai emerges as a catalyst for the synthesis of physics-based simulations with novel machine learning and AI-based methods. This interconnectedness is essential for addressing grand challenges, such as developing novel materials for building new computing platforms for AI for physics.

In conclusion, itwinai is a valuable and versatile resource, empowering researchers and scientists to embark on collaborative and innovative scientific research endeavors across diverse domains. The integration of physics-based digital twins and AI frameworks broadens possibilities for exploration and discovery through itwinai's user-friendly interface and powerful functionalities.

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