Scalable Multi-Facility Workflows for Artificial Intelligence Applications in Climate Research

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***Abstract*—Earth observation satellites and earth system models are sources of vast, multi-modal datasets that are invaluable for advancing climate and environmental research. However, their scale and complexity pose significant challenges for processing and analysis. In this paper we discuss our experiences in developing and using a scientific research application using an automated multi-facility workflow that orchestrates data collection, preprocessing, artificial intelligence (AI) inferencing, and data movement across diverse computational resources, leveraging the Advanced Computing Ecosystem Testbed at the Oak Ridge Leadership Computing Facility (OLCF). We demonstrate that our workflow can be seamlessly integrated and orchestrated, across research facilities managed by different federal agencies, to enable an AI application in order to extract new scientific insights from climate datasets using data intensive computational methods. The experimental results indicate that the multi-facility workflow significantly reduces processing time, enhances scalability, and maintains high efficiency across varying workloads. Notably, our workflow processes 12,000 high-resolution satellite images in just 44 seconds using 80 workers distributed across 10 nodes on the OLCF systems. Such high throughput is essential for dynamic tokenization and sharding of petascale satellite data for distributed AI model training and inferencing at scale across thousands of GPUs.**

***Index Terms*—satellite images, climate data, artificial intelligence, multi-facility scientific workflows**

I. Introduction

Monitoring, understanding and mitigating the impacts of climate change is one of the pressing problems being addressed by the scientific research community. Nations across the world have invested heavily in collecting data that have been synthesized into useful information for making decisions. Nevertheless, we are still faced with the challenges of deriving timely and actionable intelligence to invoke decisions with confidence across a range of spatiotemporal scales under a changing climate. Recent technological solutions involving advanced architecture, platforms and infrastructure are enabling us to adopt agile approaches toward developing and deploying applications for research, operations and decisions for climate, energy, environment and sustainability.

The climate and environmental research and operational community have assembled an arsenal of high quality data collections covering the entire planet for over a century. These data collections consist of observational datasets from earth observation (EO) satellites, in-situ measurements, and simulations by earth system models (ESM). The NASA Earth Science Data Systems (ESDS) program is anticipating a storage requirement of 600 PB by 2030 [1]. Similarly, the DOE Atmospheric Radiation Measurement (ARM) program is already managing nearly 6 PB of high quality data from 11,000 data products derived from 450+ instruments [2]. The holdings at the meteorological data archive at the European Center for Medium Range Forecasts (ECMWF) exceed 600 PB [3].

A comprehensive climate and environmental assessment necessitates the acquisition, management and analysis of distributed and disparate data collections posing logistical and technological challenges across geopolitical and organizational boundaries. Future computational ecosystems and services need to ease the burden on research scientists and decision makers in marshalling the necessary resources toward synthesizing timely results and analyses. However, the manual processes currently required to preprocess, analyze, and infer from these datasets are time-consuming and computationally intensive. These challenges underscore the urgent need for automated and autonomous solutions to harness the full potential of these diverse data assets for scientific discovery.

Processing multi-modal, distributed datasets demands a sophisticated, automated workflow capable of orchestrating data collection, movement, and processing across diverse computational resources [4], [5]. The U.S. Department of Energy's (DOE) Integrated Research Infrastructure (IRI) program addresses these challenges by providing seamless, interoperable, and reliable orchestration capabilities across its advanced science facilities [6]. By leveraging the powerful and flexible Advanced Computing Ecosystem (ACE) testbed at the Oak Ridge Leadership Computing Facility (OLCF), this paper investigates how IRI can best support the preparation, training, and inference use case with an artificial intelligence (AI) application for climate and weather research. We present a multi-facility workflow that automates the data acquisition, preprocessing, inference, and data movement tasks for petascale climate datasets, demonstrating how AI applications can be effectively deployed within this ecosystem to uncover new insights. Additionally, we provide a detailed analysis of the workflow's performance, showcasing its scalability and adaptability to meet the growing demands of climate data analytics.

This study not only advances the state-of-the-art in climate

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and environmental data analytics but also exemplifies the potential of integrating AI foundation models with advanced computing infrastructures for accelerated scientific discovery.

This paper makes the following contributions:

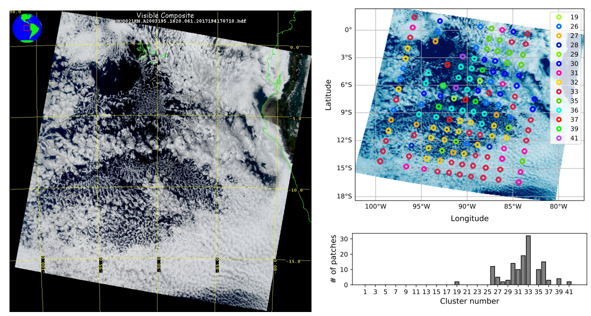
1) We present a multi-facility workflow that automates the entire lifecycle of large-scale EO and ESM data processing, including preprocessing, AI inference, and data movement.
2) We demonstrate how AI applications can be effectively integrated into this workflow to analyze petascale climate datasets, uncovering new insights that were previously challenging for many. Additionally, we highlight the workflow's user-friendly design, which simplifies the complex processes of data integration and analysis, making it more accessible to scientists and reducing the learning curve for deploying advanced computational methods.
3) We provide an in-depth analysis of the workflow's performance, highlighting its ability to scale across diverse computational environments. Our evaluation includes both strong and weak scaling tests conducted on the ACE testbed at OLCF. Results indicate that the workflow maintains high efficiency even as data volume and computational demands increase, with a linear scaling performance and consistent throughput across varying workloads. This scalability and throughput will facilitate the dynamic tokenization of petabytes of satellite data for distributed AI model training, spanning thousands of GPUs while eliminating unnecessary duplication of large data collections.

This paper is organized as follows. §II illustrates the cloud classification problem, motivating the need for seamless workflows for managing and processing multi-modal EO and ESM data and their models. §III describes how we convert the science requirements for cloud classification into an automatable workflow to be run across OLCF's advanced cyberinfrastructure. §IV presents performance results of the end-to-end workflow as well as each individual components. §V contextualizes this work in the scope of the broader IRI program. Finally, §VI presents concluding remarks.

II. Satellite Imagery for Cloud Classification through Machine Learning

The Moderate Resolution Imaging Spectroradiometer (MODIS), hosted on NASA's Aqua and Terra satellites, have been collecting visible to mid-infrared radiance data in 36 spectral bands. The Aqua satellite [7] has been in operation since 2002, and Terra [8] since 2000. Deep learning applications have been explored with various MODIS products [9], [10], demonstrating that they provide novel scientific knowledge to improve our understanding of the earth system. This wealth of data and the scientific challenges provide us a strong motivation for developing machine learning (ML) workflows that can equip the climate research community to develop a deeper understanding of the role of clouds in modulating the earth's climate system.

In this study, we examine the use of an EO machine learning (EO-ML) workflow that employs a MODIS radiance data product with an AI-enabled Rotationally Invariant Cloud Clustering (RICC) algorithm. This self-supervised deep neural network serves as an initial step towards developing a foundation model for remote sensing of clouds over oceans from MODIS data. The AI model for RICC has been initially trained on a dataset of 1 million images. It combines a rotationally invariant autoencoder with agglomerative hierarchical clustering [11] that clusters cloud patterns and textures from MODIS imagery, grouping similar cloud textures and physical properties into the same class by using only Level-1B (L1B) multispectral MODIS imagery as input without reliance on location, time/season, and pre-designated class definitions. Leveraging the capability of RICC, the AI-driven Cloud Classification Atlas (AICCA) [12] provides 42 cloud classes, which are derived from clusters of 24 years of cloud imagery over the ocean from both the MODIS instruments.



(a) (b)

Fig. 1: (**a**) MODIS true color swath image off the west coast of South America from the Terra instrument between 18° S to 3° N, 76° W to 104° W, observed on 14 July 2003. Image acquired from Level-1 and Atmosphere Archive and Distribution System; (**b**) MODIS swath (a) with 133 ocean-cloud tiles represented by a dot with color indicating its associated one of 42 AICCA class labels. AICCA dataset groups spatially coherent and visually similar textures of cloud tiles into the same class. AICCA classes seen in (a) identify stratocumulus clouds into multiple classes and separate subtle spatial differences.

A. MODIS Data Collection

The MODIS instruments collect data over approximately 2330 km by 2030 km *swath* across 36 spectral bands of range 0.4–14.4 μm. The observations are binned every five minutes into image granules (scenes). NASA processes MODIS data to create various derived products and stores at the Level 1 and Atmosphere Archive and Distribution System Distributed Active Archive Center (LAADS DAAC). LAADS DAAC offers multiple quick and easy-access web interface services. The data collection we are using is from the MODIS L1B calibrated radiances (MOD021KM/MYD021KM, hereafter MOD02) and Atmosphere L2 cloud product (MOD06L2/MYD06L2, hearafter

MOD06). MOD03/MYD03 [13], [14] (hereafter MOD03) products provide latitude and longitude metadata for their geolocation. (Note that MOD and MYD are used to distinguish products between Terra and Aqua, respectively.)

B. AICCA: AI-driven Cloud Classification Atlas

AICCA provides 42 AI-generated cloud class labels for all 128×128 pixel (∼100 km by 100 km) ocean cloud *tiles*, a smaller unit of image of 128 × 128 pixels × 6 channels, sampled by radiances from MOD02 product over the 24 years of MODIS data archives. Applying the RICC method [11] to MOD02 product, ocean cloud tiles are assigned among one of 42 cloud classes as shown in Fig. 1. The data production uses selected derived physical properties, spatiotemporal information, and metadata from the MOD06 product to derive associations between AICCA cloud classes, cloud physical properties, and other EO/ESM datasets in a daily to decadal climate analysis.

The original AICCA label creation workflow comprises of four principal stages (See Fig. 1 in [12]) as follows: **(1) Data acqusition and preparation**: Download MODIS products from the NASA LAADS DAAC via HTTPS download scripts accelerated by FuncX [15] and Globus service [16] for the retrieval of 850TB of three different MODIS products between 2000–2023, and store the downloaded data on a shared filesystem at an HPC facility. As described in Section II-A, select specific bands from MOD02 and subdivide each swath into non-overlapping 128×128 pixel tiles. The data curation process conducts ocean cloud tile selection defined as $> 30\%$ cloud pixels over only ocean regions. **(2) RICC training**: Train RICC algorithm over 1M tiles and apply clustering of those latent representations to generate cluster centroids. **(3) Cluster evaluation**: Evaluate resultant clusters quality based on their protocol. **(4) Label assignment**: With the trained autoencoder and centroids, predict cloud labels and calculate physical properties and other metadata information for each tile for unseen data. The Parsl parallel Python library [17] efficiently scales this inference process across hundreds of CPU nodes, enabling the generation of the AICCA dataset in NetCDF format with high throughput and consistency.

While components of the original workflow were scaled using Globus computing libraries (i.e., FuncX and Parsl), it continued to depend on manual processes and lacked integration across the four stages. It is essential to unify these stages into an automated workflow service For seamless scalability and deployment.

III. Automated Workflow Integration for Cloud Classification in the ACE IRI Ecosystem

In this section, we present an automated EO-ML workflow, executed on OLCF's ACE IRI infrastructure, designed to automate and integrate the previously disconnected, labor-intensive steps required for cloud classification across a continuum of computing resources. These tasks, when performed manually, are not only time-consuming but also prone to inconsistencies and human error. Our workflow transforms these ad hoc, human-powered processes into an efficient, reusable pipeline, as depicted in Fig. 2. It is organized into five essential components: (1) downloading data from NASA LAADS DAAC onto the file system on ACE Defiant; (2) preprocessing images to isolate ocean cloud pixels; (3) automatically triggering an inference script on the preprocessed tiles; (4) performing unsupervised inference; and (5) transferring the results to Frontier for large-scale climate analysis.

Specialized software is required to programmatically link and automate the various data and computing elements of the original EO-ML workflow. This software not only coordinates data transfer and compute tasks but also dynamically orchestrates these tasks based on workflow events. In order to achieve this, we leverage the Globus software tools ecosystem, including Globus Transfer [18] for secure and efficient data movement, Globus Compute [15] and Parsl [17] for remote and local execution of computations on heterogeneous infrastructure, and Globus Flows [19] for defining, executing, and monitoring complex workflows.

In the following, we detail how we specifically configure and use each tool as part of the EO-ML workflow:

(1) Data download: NASA's LAADS DAAC provides access to its data via HTTPS, requiring clients to manage transfers using common request libraries such as wget. Users can specify a time span, ranging from a single day to up to 24 years, covering the entire archive of MODIS data available in LAADS, as well as select specific MODIS products from the Aqua or Terra satellites (e.g., MOD021KM). Each day's dataset can contain up to 288 files, with typical sizes of approximately 32GB for MOD02, 8.4GB for MOD03, and 18GB for MOD06, making parallel downloads essential for handling larger data volumes efficiently.

To automate the retrieval of these files to the compute resources, we implemented a remotely executable Globus Compute function. In this setup, users configure their workflow through a locally available YAML file for their queries, specifying their compute endpoint, LAADS credentials, MODIS product, time span, and local paths to save the desired data products. The downloads for each time span can be distributed across multiple Compute workers to maximize bandwidth utilization. Once retrieved, files are stored in local directories. If a worker completes its download task and additional time spans are queued, it automatically begins the next task. If no further tasks are available, the worker gracefully terminates.

(2) Preprocess: Preprocessing is one of the most resource-intensive and highly parallelizable components of our EO-ML workflow. During this step, raw swath images are transformed into uniformly-sized tiles, each containing cloud images with multiple channels. We package preprocessing into a single script that subdivides each 2030 pixels × 1354 pixels × 36 channels MODIS swath into a set of 128 pixels × 128 pixels × 6 channels 'tiles'. The script is designed to ensure that each tile exclusively contains ocean or cloud pixels.

Tile creation is performed independently for each swath image across various time stamps and involves integrating data from three distinct MODIS products at each time step:

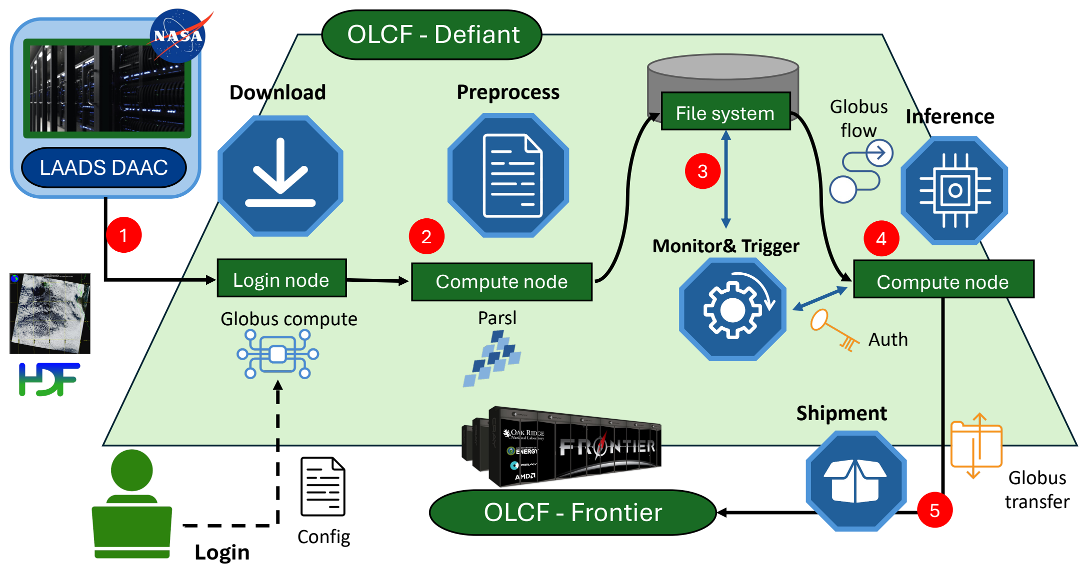


Fig. 2: The earth observation ML workflow automates the four data processing stages under the Globus software ecosystem. (a number with a red circle highlights each step.) To initiate the workflow the user defines configuration in a YAML file. **(1) Download**: Download the set of MODIS products from the respective NASA Distributed Active Archive Center (DAAC). Globus compute automates the download and populated data on the OLCF ACE Defiant system. **(2): Preprocess**: Preprocessing script decomposes 2030 pixels $\times$ 1354 pixels $\times$ 36 channels MODIS swath image into a set of 128 pixels $\times$ 128 pixels $\times$ 6 channels image 'tiles' and selects the tiles over oceans only. Parsl efficiently scales the preprocessing with multi-workers across multi-nodes. **(3) Monitor & Trigger**: a monitoring script scans whether preprocessed files are generated and stored in file system. If yes, triggers the inference script. **(4) Inference**: Inference predicts one of 42 AICCA cloud classes. **(5) Shipment**: Finally, labeled data created from the inference stage is transferred to the lustre file system on Frontier for downstream analytics, including training of new foundation models.

MOD02, MOD03, and MOD06. Our script leverages metadata from each product (e.g., cloud and ocean pixel locations) to exclude tiles with land pixels and restrict tiles to those containing at least 30% ocean pixels. This process ensures the creation of more effective tiles for deep learning training [11].

To parallelize preprocessing on Defiant, we configure a Parsl Slurm provider to automatically allocate blocks of compute nodes, with each node containing a configurable number of Parsl workers. To avoid HDF read errors that can occur from partially reading files, preprocessing is delayed until all downloads are complete. Once Parsl successfully allocates nodes, it handles the distribution of tasks to workers and monitors their completion. It is important to note that processing time can vary depending on the proportion of ocean and land pixels, as well as the availability of certain information bands during nighttime hours. Finally, each Parsl worker saves the processed files as NetCDFs.

(3) Monitor & Trigger Cloud label prediction using RICC model can be performed asynchronously with NetCDF file generation. As such, we divide the task of splitting the inference process into two parts: (i) monitoring the file system for the creation of new files, and (ii) triggering the inference. These steps are automated using a Globus Flow:

- Launch file system crawler to identify new files.
- Perform inference using Tensorflow script.
- Append cloud labels to NetCDF file.
- Move updated NetCDF file to transfer-out directory.

Once the Flow processes all NetCDF files, the workflow is ready for the final step.

(5) Shipment: In this final step, the NetCDF files, now enriched with the derived classifications, are transferred to Frontier's Orion shared file system via Globus Transfer. Once in place, these files are readily accessible for research scientists and downstream workflows for further analysis.

IV. Demonstrations

In this section, we evaluate our EO-ML workflow by evaluating the collective and individual latency of workflow steps, the scalability of preprocessing image tiles, and the overall ease of use for a scientist intending to create and execute this workflow. For this benchmarking experiment, we select cloud images observed by the MODIS Terra instrument on January 1st, 2022. For most experiments, we use OLCF's 36-node Defiant cluster. Each compute node contains a 64-core AMD EPYC 7662 CPU each with 256GB DDR4 RAM, and linked to four AMD MI100 GPUs. Nodes are linked via a 12.5 GB/s Slingshot-10 interconnect, and a 1.6PB Lustre file system.

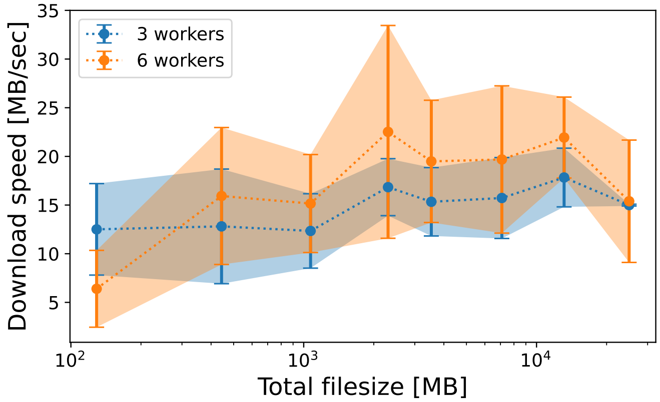


Fig. 3: Download speed statistics with 3 workers (blue) and 6 workers (orange) for different MODIS product sizes. Dots represent mean speeds; shading shows standard deviation.

A. Downloading

The first step of ML pipelines with EO and ESM datasets generally starts with downloading these datasets, which are publicly available from different institutes and public clouds, to employ HPC resources for AI model training and inference. Again, our test application requires three different products: MOD02, MOD03, MOD06 (see detail in Section II). We assess performance by average download speed per second across various file sizes starting from 100MB (i.e., one file per product) to 30GB (i.e., about 128 files per product) as shown in Fig. 3. We conduct three iterations for cases deploying 3 and 6 workers, respectively, to evaluate the range of downloading performance. Increasing the number of download workers boosts the average download speeds by an average of 3 MB/sec, except when downloading a single file for overheads.

B. Preprocessing: scale

After completing the downloads, our workflow leverages Parsl to scale the conversion of raw product images into smaller tiles optimized for ML inference. We assess strong and weak scaling performance by varying the number of workers and nodes, iterating each data point five times.

We examine the strong scaling performance across workers. Processing a fixed set of 128 MOD02 files, we measure completion time while doubling the number of workers from 1 to 128. Notably, the increase from 64 to 128 workers requires the use of a second node. Next, we assess strong scaling performance across nodes. In this scenario, we fix the number of MOD02 files at 80, with each node running 8 workers, and then sequentially scale the number of nodes from 1 to 10. The results of both worker and node scaling are presented in Fig. 4. We observe near-linear strong scaling performance with an increasing number of nodes (Fig. 4b), and sub-linear scaling when increasing the number of workers on a single node (Fig. 4a), indicating significant on-node resource contention.

We then evaluate weak scaling performance by varying the number of nodes and workers, assigning an equal number of files (n=2) to each worker in Fig. 5. Consistent with the strong scaling results, we observe excellent performance when increasing the number of nodes (Fig. 5b), but encounter resource contention when scaling up the number of workers within a single node (Fig. 5a).

In summary, the preprocessing step of our EO-ML workflow achieves optimal scaling by increasing the number of nodes.

TABLE I: Throughput of MODIS 128 pixels × 128 pixels tile under four scaling experiment.

Strong scaling			
# workers	**# tile per sec**	**# nodes**	**# tile per sec**
1	10.52	1	36.05
2	18.10	2	73.25
4	25.01	3	98.73
8	36.59	4	135.42
16	38.74	5	177.69
32	37.95	6	192.32
64	37.34	7	196.70
128	71.01	8	216.86
-	-	9	264.13
-	-	10	267.44
Weak scaling			
# workers	**# tile per sec**	**# nodes**	**# tile per sec**
1	21.32	1	32.82
2	25.87	2	69.34
4	27.23	3	100.36
8	27.48	4	126.62
16	32.73	5	165.12
32	31.09	6	175.61
64	35.36	7	196.81
128	67.69	8	188.88
-	-	9	197.26
-	-	10	271.68

C. Preprocessing: throughput

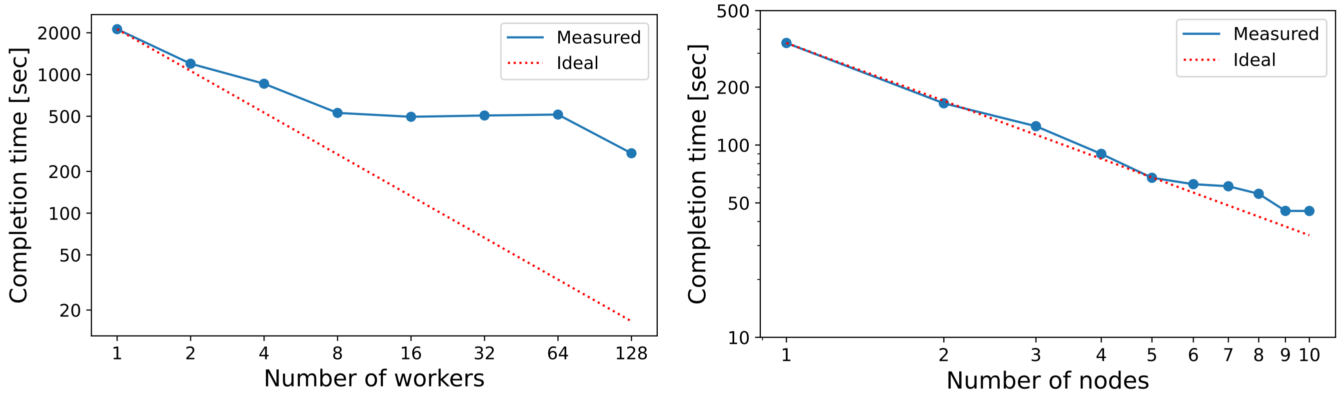
In deep learning applications, data preprocessing must prioritize high throughput due to the large-scale training and inference datasets that must be efficiently prepared. In our experiment, we define 'throughput' as the number of tiles processed by our preprocessing application per second.

Table I summarizes the throughput results under various worker and node counts. During the strong scaling experiments, we achieved a peak throughput of approximately 267.44 tiles per second. In contrast, the weak scaling experiments showed a slightly higher maximum throughput of 271.68 tiles per second, surpassing the strong scaling result by roughly 4 tiles per second.

These findings indicate that while both strong and weak scaling can deliver high throughput, weak scaling offers a slight advantage in maximizing data processing efficiency.

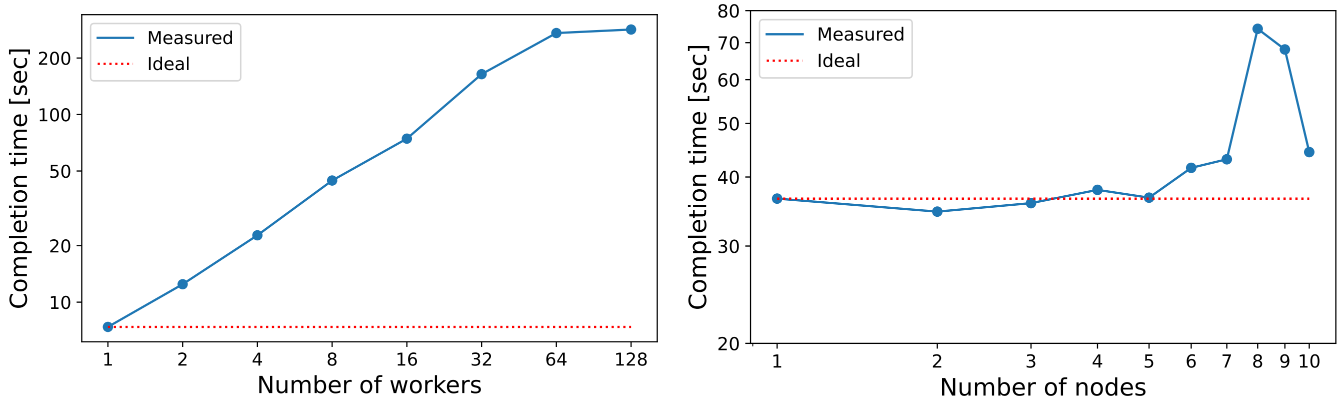
D. Dynamic workflow resource allocation

The key advantage of an automated workflow lies in its ability to adaptively manage resource allocation at each step. As illustrated in Fig. 6, 3 workers are assigned to download products, 32 workers to preprocessing, and 1 worker to inference. The time series of active worker counts shows that the workflow (1) increases resource allocation after completing the network-intensive, compute-light download task and begins



(a) (b)

Fig. 4: Plots of completion time by strong scaling experiment as a function of (a) the number of workers and (b) the number of nodes.



(a) (b)

Fig. 5: Similar to Fig. 4, we plot the completion time by weak scaling experiment as a function of (a) the number of workers and (b) the number of nodes.

the compute-intensive, parallelizable preprocessing step, (2) dynamically scales down resources as workers complete their tasks, and (3) efficiently allocates resources to different tasks concurrently, with inference starting before preprocessing is fully complete. Overall, our EO-ML workflow achieves flexible resource management by scaling to accommodate the unique needs of each workflow step, which has not been demonstrated in other EO-ML studies.

Finally, we examine the average flow latency and communication time between workflow components. As shown in Fig. 7, we observe that the download step launches workers with Globus Compute, establishes a connection to the LAADS server, and configure the list of files to be downloaded in just 5.63s. As there is no data transfer before preprocessing, preprocessing (i.e., tile creation) begins quickly thereafter, and takes 32.80s. The preprocessing latency includes starting Parsl, the Slurm scheduler allocating nodes, and the tile creation itself. It excludes the queue wait time and the minuscule communication overhead of Parsl workers. Finally, our monitor crawler asynchronously connects to our inference pipeline orchestrated with Globus Flow. Once the Flow instance is created, the overhead becomes extremely fast, with latency requiring the action to move execution and termination at approximately 50 milliseconds. This extremely fast overhead time is also evident in Fig. 6, where the green worker scales in and out in very small duration. We leave the optimization of the suboptimal communication flow between preprocess and inference in future work.

V. Discussion: IRI Ecosystem for Breakthrough Science

In recent years, the planet has experienced an increase in the rate of surface warming. This has been aided in part by the decrease of aerosols over the oceans that allowed more sunlight to reach the surface of the earth [20]. But under the current growth and emission scenario the current rate of warming will gradually slow down but the climate and environmental impacts of this warming will continue to grow for a longer period of time [21], contributing to extreme events

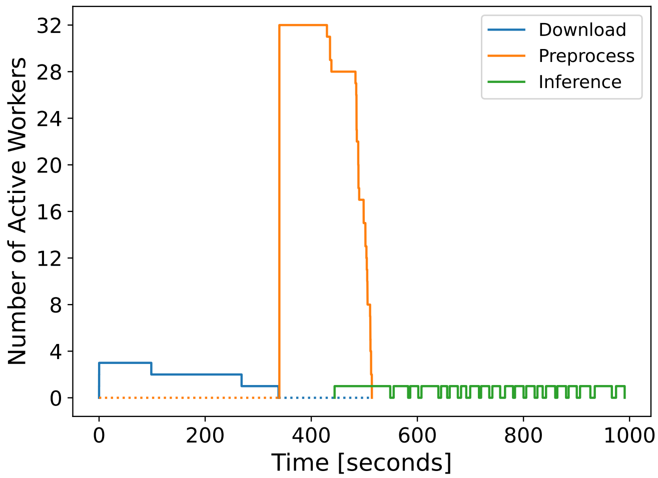


Fig. 6: An example automation timeline. Blue line depicts download step, orange represents patch creation, and green is inference process.

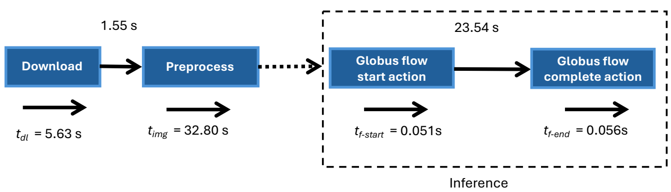


Fig. 7: An illustration of EO-ML workflow breakdown across all workflow process (boxes). Solid arrows between boxes show the data communication latency and arrows under the boxes represent the latency involved in launching a job and starting the process. Dashed arrow is an asynchronous connection, and this gap is inconsequential to our workflow.

in different parts of the world [22]. Predicting, monitoring, and responding to extreme events require research and operational infrastructure to support timely decisions, which will involve the integration of: (1) earth observations from satellites and in-situ observation systems that continually stream data; (2) methods and algorithms, including numerical models and AI applications, to synthesize data to environmental situational awareness and actionable information; and (3) mechanisms to make and invoke decisions. The ongoing computational campaign would involve the assimilation of streaming data into simulations and data intensive AI applications including digital twins of the earth. The DOE Integrated Research Infrastructure will offer such visionary capabilities to realize breakthrough science and decisions.

The nature and distribution of clouds, their properties and climate feedback are the sources of major uncertainties in our understanding of the earth's climate system [23]. Here we have demonstrated the utility of the ACE IRI Testbed in seamlessly accomplishing the scientific task of classifying different cloud types over the oceans and monitoring their changes over decades using an AI application based on satellite data from the NASA MODIS instruments. The enduring nature of earth observation missions require that AI applications are continually trained periodically on new data without catastrophically forgetting what had been learned previously [24] while at the same time new data are used to understand how the earth system may be responding to the changing climate. In the future we plan to extend our current workflow and services to support more dynamic AI applications that involve training new versions of the models, continual learning and inferring with batch as well as streaming data. The ML pipeline will evolve to facilitate model merging, data efficient learning while minimizing the carbon footprint of the climate research activities on the IRI.

The advent of AI foundation models offers new opportunities to deliver breakthrough science even more efficiently. Foundation models, pretrained on a very large volume of data, can be further adapted for a host of new tasks and applications via fine tuning, requiring relatively less amount of data. The OLCF ACE IRI Testbed will continue to evolve to support MLops involving the adaptation of FMs for novel new applications. For example, the pretrained science FM, based on the MODIS atmospheric data, can be further adapted with multimodal data from earth system models to develop AI surrogate models that can be incorporated into earth systems models to improve the fidelity of the models or to further accelerate the simulations for quicker time to solutions.

A. Advancing integration with the IRI ecosystem

At a more technical level, we also envision a future when the IRI can implement a federated pipeline-as-a-service platform that offers a shareable and publicly accessible repository of complete workflows or individual workflow steps, which can be customized with various components from a community-driven pipeline service. Many scientific communities now publicly share their ML codebases; yet challenges arise when users re-implement portions of these pipelines. A federated orchestrated pipeline service mitigates this issue by enabling the entire or subset of pipeline to be registered as executable and shareable functions, thereby minimizing access barriers and streamlining usage for all science users ultimately beyond boundaries of science communities. Establishing community standards for developing seamless, shareable, and reproducible ML pipelines is crucial. This approach democratizes access, accommodating users of varying levels of expertise and familiarity with the data. Overall, developing robust community standards for designing ML pipelines that are both reusable and reproducible will be essential for advancing the field.

To enhance accessibility for domain scientists, our goal is to enable users to define, customize, and execute EO-ML workflows using high-level languages like the Common Workflow Language (CWL) [25] or Globus Flows. Currently, the Parsl component requires manual initiation on local resources, which hinders seamless execution. To address this, we plan to use the Zambeze [26] orchestration framework to facilitate remote configuration, invocation, and monitoring of workflow components, simplifying user interaction. However, the workflow orchestration across DOE computing facilities (OLCF, NERSC, ALCF) is fragmented, with each using different systems. To achieve interoperability, our strategy involves aligning these systems for seamless data and resource sharing [27]. In the near term, we will focus on manual user authentication, credential management, and developing adapters for cross-facility communication.

Finally, to ensure reusability and reproducibility within the IRI ecosystem, we will integrate advanced provenance tracking and telemetry tools for real-time workflow insights. By publishing clear input and output schemas for each workflow component, we aim to minimize errors and support the creation of reliable, reusable workflows that can be consistently reproduced across different computational environments.

VI. Conclusion

The Oak Ridge Leadership Computing Facility, home to the ACE IRI testbed and the world's fastest supercomputer, Frontier, is poised to significantly advance the development of multi-facility workflows that leverage large-scale earth observation and climate model datasets. Our preliminary efforts with the EO-ML workflow demonstrate the potential of integrating self-supervised deep learning techniques with automated workflows to process petascale MODIS imagery datasets effectively. In this paper, we discussed a pipeline by which domain scientists can easily deploy machine learning workflows across diverse cyberinfrastructure. To illustrate our approach, we leverage several Globus services to construct our workflow, and we anticipate further enhancements with the adoption of tools like Zambeze. Looking ahead, continually leveraging IRI advances in connecting the vast computing resources of DOE facilities of these workflows will maximize the available power for climate science and earth observation, paving the way for more easy-to-use, scalable, and reproducible/reusable analyses.

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