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HPC Ontology: Towards a Unified Ontology for Managing Training Datasets and AI Models for High-Performance Computing

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***Abstract*—Machine learning (ML) techniques have been widely studied to address various challenges of productively and efficiently running large-scale scientific applications on heterogeneous supercomputers. However, it is extremely difficult to generate, access, and maintain training datasets and AI models to accelerate ML-based research. The Future of Research Communications and e-Scholarship has proposed the FAIR data principles describing Findability, Accessibility, Interoperability, and Reusability. In this paper, we present our ongoing work of designing an ontology for high-performance computing (named HPC ontology) in order to make training datasets and AI models FAIR. Our ontology provides controlled vocabularies, explicit semantics, and formal knowledge representations. Our design uses an extensible two-level pattern, capturing both high-level meta information and low-level data content for software, hardware, experiments, workflows, training datasets, AI models, and so on. Preliminary evaluation shows that HPC ontology is effective to annotate selected data and support a set of SPARQL queries.**

***Index Terms*—Ontology, HPC, FAIR, datasets, AI models**

I. Introduction

Due to the extreme heterogeneity and complexity of high-performance computing (HPC) node architectures, white-box analytical modeling techniques have become less tractable for analyzing and optimizing large-scale scientific applications. As an alternative, Artificial Intelligence (AI), especially machine learning (ML)-based techniques have been widely used to address various challenges in HPC, including those related to performance modeling and prediction [1]–[4], performance analysis [5]–[9], resilience [10], [11], data storage format selection [12], memory optimization [13], scheduling [14], and so on.

However, the HPC community's consensus is that it is difficult to find, access, prepare, share, and reuse high-quality training datasets and AI models, as stated by a recent report of the Department of Energy's Office of Science [15]. This is especially true when ML is applied to analyze and optimize large-scale HPC applications running on heterogeneous node architectures. Researchers spend a significant amount of effort using highly specialized tools (including compilers, performance tools, and runtime systems) to extract and process training datasets from HPC systems. A range of machine learning frameworks is then used to generate AI models. Such datasets and AI models are stored in numerous formats, often without sufficient metadata to describe their semantics. Many datasets and models are underutilized. Part of the reason is that the community has not established standard processes to share the valuable datasets and the corresponding AI models. As a result, researchers and developers have to resort to costly repeated data collection processes. The HPC community cannot quickly build, evaluate, and reuse machine learning techniques to address pressing HPC challenges.

The problem the HPC community is facing is not unique. In many other research communities, researchers are establishing standard guidelines and recommending best practices to make scientific data Findable, Accessible, Interoperable, and Reusable (FAIR) [16]. Briefly, Findability means that data can be found online, typically through indexing in search engines. Accessibility indicates that data can be retrieved directly or via an approval process. Interoperability means that data follows standards. Finally, reusability denotes that the context of data generated (metadata) is documented so it can be compared to or integrated with other datasets.

This paper focuses on our preliminary work of developing a core component to enable FAIRness of training datasets and AI models for HPC: the HPC ontology, which is a collection of essential concepts and properties capturing information in the domain of HPC, using formal knowledge representation of Web Ontology Language (OWL) [17]. The HPC ontology provides a common vocabulary to describe various datasets and AI models. It also provides the semantics to enable the interoperability of heterogeneous data. In particular, we make the following contributions.

- We analyze the FAIR data principles and identify ontologies as essential enabling components.
- We create a set of guidelines for designing the HPC ontology, which takes into consideration the special requirements and constraints of making datasets and AI models FAIR in the HPC community.
- A high-level core ontology is designed to provide stan-

dard concepts and properties to annotate datasets, and AI models. This is required to facilitate data sharing and searching.
- A set of low-level supplemental components are presented to capture fine-grained information in various subdomains such as computers and performance datasets.
- Using a few use cases, we evaluate the benefits of the HPC ontology for annotating data and answer queries.

The remainder of this paper is organized as follows. In the next section, we will introduce the background information about the FAIR principles and the critical roles of ontologies. Section III presents the design philosophy of the HPC ontology. Section IV details the high-level concepts and properties of the HPC ontology, while Section V explains how more fine-grained information is organized in low-level components for various subdomains. We evaluate the current draft HPC ontology in Section VI. Related work is discussed in Section VII. Finally, Section VIII concludes the paper with a plan for future work.

II. Background

We provide background information about the FAIR principles for sharing scientific data and how ontologies play an important role in achieving FAIRness.

A. The FAIR Data Principles

Accelerating scientific discoveries and innovations depend on a good ecosystem managing experiment data for various purposes such as validation and reusing. Unfortunately, existing scholar publication systems focus mostly on papers. The associated experiment data is either discarded or treated as a secondary citizen with lower standards for publishing. In response to the urgent need in the scientific community to improve the infrastructure supporting the reuse of scholarly data, the Future of Research Communications and e-Scholarship (FORCE11) proposed the FAIR data principles [16] describing four fundamental principles: Findability, Accessibility, Interoperability, and Reusability. These principles are further refined, as shown in Table I.

TABLE I
FAIR Principles proposed by FORCE11 [16]

F: To be Findable	
F1	(Meta)data are assigned a globally unique and persistent identifier
F2	Data are described with rich metadata
F3	Metadata clearly and explicitly include the identifier of the data they describe
F4	(Meta)data are registered or indexed in a searchable resource
A: To be Accessible	
A1	(Meta)data are retrievable by their identifier using a standardised communications protocol
A1.1	The protocol is open, free, and universally implementable
A1.2	The protocol allows for an authentication and authorisation procedure, where necessary
A2	Metadata are accessible, even when the data are no longer available
I: To be Interoperable	
I1	(Meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation
I2	(Meta)data use vocabularies that follow FAIR principles
I3	(Meta)data include qualified references to other (meta)data
R: To be Reusable	
R1	(Meta)data are richly described with a plurality of accurate and relevant attributes
R1.1	(Meta)data are released with a clear and accessible data usage license
R1.2	(Meta)data are associated with detailed provenance
R1.3	(Meta)data meet domain-relevant community standards

One of the main goals of the FAIR principles is to achieve machine-actionability in order to process the large amount of scholar data generated daily. This means that data management systems should provide rich and standard information such as the type of digital objects, their formats, licensing, and appropriate operations on them. To be practical, both contextual metadata surrounding a digital object and the content of the digital object should use controlled vocabularies, which in turn are associated with controlled semantics. As a result, several refined FAIR principles shown in Table I explicitly mention vocabularies (I2), knowledge representation (I1), and community standards (R1.3) to improve machine-actionability.

B. Ontologies

Ontologies can provide the much-needed controlled vocabularies, knowledge representation, and standards to implement the FAIR data principles. Ontology [18] is a concept originating in Philosophy, referring to the study of the nature of being, as well as the basic categories of them and their relations. In recent decades, it has become a formal way to explicitly represent knowledge in a domain. An ontology [18], [19] is a formal specification for explicitly representing knowledge about types, properties, and interrelationships of the entities in a domain. It provides a common vocabulary to represent and share domain concepts. Compared to tree-like taxonomy solely modeling the generalization-specialization relation, an ontology can form a much more complex graph with edges to model any kinds of relationships between entities (represented as graph nodes). Such graphs are often called knowledge graphs in many communities.

Figure 1 illustrates an example ontology for Robotics. Each node in the graph represents a concept or instance, and each edge carries a property indicating the relations between the two nodes it connects. For example, there are two nodes named "Agent" and "Object" indicating two concepts (or classes). The "is-a" edge between them means that one is a subclass of the other. An edge labeled 'instanceOf" denotes that a node is an instance of a node representing a class. Another edge (labeled "hasPart") between "Robot" and "Arm" indicates that the latter is a part of the former.

A formal language for expressing ontologies is the Web Ontology Language (OWL) [17]. OWL is based on the description logic (DL) and is expressive enough for building sophisticated knowledge bases while still supporting efficient inference. Resource Description Framework (RDF) is a fundamental format used to store a wide range of information, including ontologies written in OWL. Each piece of knowledge

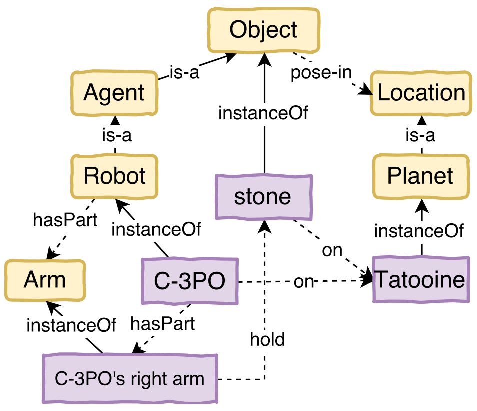


Fig. 1. An example ontology on robotics.

stored in RDF is represented as a triple, *(subject, property, object)*. For instance, *("Tatooine", instanceOf, "Planet")* states that *Tatooine* is an instance of *Planet*.

An ontology can be queried using a standard RDF query language named SPARQL. An example query in Listing 1 can be used to find all robots on the Tatooine planet using the Robotics ontology through the join of two properties. *rdf:type* is a standard RDF property to link a resource as an instance to its class. *:on* is the property to link a resource to its location.

Listing 1. Example SPARQL Query on the Robotics Ontology

```
SELECT ?s
WHERE { ?s rdf:type :Robot .
        ?s :on :Tatooine }
```

Numerous ontologies or controlled vocabularies have been developed to enhance interoperability and reusability of data in different domains. For example, EDAM [20] is an ontology for bioinformatics operations and data types. Schema.org [21] is designed to improve the interoperability of web data. The Genomic Data Commons of National Cancer Institute [22] maintains standard terms and references to public ontologies and vocabularies in dictionary files to share linked clinical and genomic data. Brick [23] is an ontology to capture the common terms and relations in the domain of smart buildings.

In summary, the use of ontologies ensures "I"nteroperability and "R"eusability of the FAIR principles. In the context of making HPC training datasets and AI models FAIR, a supportive ontology is a natural prerequisite to provide a standard vocabulary of the HPC domain. However, there is a lack of effort of creating ontologies for the domain of machine learning-based program analysis and optimizations in high-performance computing (HPC). The focus of this paper is to contribute a design of such an ontology, namely HPC ontology.

III. Design Philosophy

In order to support datasets and AI models used for HPC software analysis and optimizations, the HPC ontology has to cover a sufficiently large scope, including software, hardware, their interactions, as well as AI models. Developing a full-scale ontology to capture everything in HPC is impractical. It is also against the very idea of controlled vocabulary. There is also a choice between developing an ontology from scratch and reusing existing ones. The key to the success of a domain-specific ontology is to have a carefully controlled scope so it is easy for users to learn while covering sufficient concepts and relationships of the selected domain. With these constraints in mind, we adopt a modular design with a two-level structure for the HPC ontology, with the following design principles.

a) Principle 1: We decide to have a set of high-level core components within the HPC ontology to capture high-level concepts and relationships used to describe entire datasets or AI models. This core ontology aims to provide metadata for users to annotate datasets and AI models as a whole. The metadata may include descriptive, administrative, and statistical information about datasets and models. We expect the high-level components are mostly stable for enhanced interoperability.

b) Principle 2: A set of low-level components are developed for representing fine-grain, internal information of various subdomains. These low-level components of the HPC ontology provide concepts and relationships details for smaller domains, such as program analyses, compilers, hardware features, performance tools, and their results, libraries, SDKs, AI models, and so on. The set of low-level components is extensible to accommodate the rapid evolvement of HPC software and hardware. They can be easily added, loaded, or phased out as supplemental components to the HPC ontology.

c) Principle 3: The reality is that most HPC researchers and developers are not familiar with ontology techniques. To make the HPC ontology easy to learn, we keep the core concepts and properties of the HPC Ontology into a single namespace (with a prefix named *hpc:*), without depending on names from other ontologies. This will relieve users from the burden of learning tens of other ontologies before they can use the HPC ontology to annotate basic data or form common queries.

d) Principle 4: For particular subdomains, if there are existing high-quality ontologies that are lightweight and easy to learn, we directly incorporate them as low-level, supplemental components. For instance, to encode content of scientific datasets, we have found that providing accurate unit information is indispensable. One example is execution duration. There are multiple units used in the field, such as seconds, milliseconds, microseconds and so on. After surveying the literature, we have found that the QUDT (Quantities, Units, Dimensions and Types) ontologies, originally developed by NASA researchers, already provide a good solution for encoding data with different units of measures. It also provides a mechanism to add extensions. Therefore, we directly use QUDT to encode units of scientific data.

e) Principle 5: To enable interoperability, we also link the content of HPC ontology with equivalent concepts and relationships from mainstream ontologies, such as Dublin Core metadata [24], Schema.org [21] and DBpedia [25]. Users who are already familiar with other ontologies can still use the same terms. SPARQL query engines can easily process queries using popular vocabularies. This makes datasets and AI models annotated by HPC ontology part of the linked data ecosystem.

f) Principle 6: Although there is some progress for techniques used to automatically generate ontologies, they are still immature. We decided to create the content of the HPC ontology manually. This will give us more control over the set of concepts and relationships to be included or excluded. We can also curate the class hierarchies of different subdomains, leveraging the extensive human experiences of our team in HPC.

g) Principle 7: We use an incremental and use case driven approach to develop the HPC ontology. The initial version will be developed using a set of simple use cases. Later versions will be developed with increasingly more complex use cases combined with more strict evaluation criteria including size, completeness, accuracy, consistency, correctness, conformity to community standards, persistence, accessibility, and so on.

IV. High-Level Core Ontology

In this section, we present representative high-level concepts and their corresponding properties of the HPC ontology.

A. Basic Scenario and Naming Convention

A basic scenario described by the HPC ontology is that *some people who are members of a project used some software and hardware to conduct some experiments, which in turn used some input data to generate training datasets or AI models*. The semantics can be mapped to three high-level concepts, including Agent, Activity, and Artifact. Essentially, *some Agent conducted some Activity which used some Artifact as input and generated some other Artifact*.

As shown in Figure 2, we follow a common naming convention when defining vocabularies in the HPC ontology: Singular nouns in CamelCase are used to indicate a Class. Multiword names are written without any spaces but with each word written in uppercase. Relationship (or Property) names start with lowercase letters. For example, *hpc:Project* means a class while *hpc:project* indicates a property that links some data with its associated project.

Dashed arrows in the figure indicate the *isA* relation between a subclass and its superclass. For instance, both training datasets and AI models are kind of data in this context. Solid line arrows indicate other relationships. Some arrows have only a single label to denote a single relationship. To simplify the diagram, inverse relationships are combined in a single arrow with a pair of relationship labels. For example, the label of the arrow between Person and Project includes both *hpc:memberOf* and *hpc:member*. Not all edges are shown in the figure to avoid a cluttered figure.

B. Top level Concept: Thing

To provide provenance of all information, the very top level concept in the HPC ontology, *hpc:Thing*, is associated with a set of fundamental properties (listed in Table II) about its unified resource identifier, the type of the ID (such as Open Researcher and Contributor ID and Digital Object Identifier), name, URL, etc. Any other concepts (from both high and low levels) are direct or indirect subclasses of *hpc:Thing*. They naturally inherit all the fundamental properties of *hpc:Thing*. The *hpc:Thing* node and its edges are not shown in Figure 2 to simplify the figure.

TABLE II
Properties of the Thing Class

Property	Data-type	Description
hpc:id	xsd:anyURI	URI of the thing
hpc:idType	xsd:string	Type of the ID, such as ORCID, DOI, etc.
hpc:name	xsd:string	Name of the thing
hpc:alternateName	xsd:string	An alias for this item
hpc:description	xsd:string	Short description
hpc:url	xsd:anyURI	URL of the official website of a thing
hpc:submitter	xsd:anyURI	Who submits this piece of info.
hpc:submitDate	xsd:dateTime	Date of submission

C. Activity and Experiment

As shown in Figure 2, the centerpiece of this design is the concept of Activity, which connects to many other concepts through properties such as *hpc:used*, *hpc:generated*, *hpc:wasAssociatedWithSoftware*, *hpc:usedWorkflow*, *hpc:wasConductedBy*, and so on. An activity is something that occurs over a period of time. An activity could happen after another one, linked using *hpc:wasPrecededBy*. Experiment is a subclass of Activity to represent HPC experiments.

Table III lists major properties of the Experiment class. For convenience, we also define equivalent properties as needed. For example, *hpc:used* is the same as *hpc:hadInput*. *hpc:wasAWS* is a short name for *hpc:wasAssociatedWithSoftware*. *hpc:wasAWS* is equivalent to *hpc:wasAssociatedWithHardware*. There is also the *wasPrecededBy* property to link a sequence of experiments.

TABLE III
Major Properties of the Experiment Class

HPC Ontology Property	Data-type	Description
hpc:used	xsd:anyURI	Input data, ==hpc:hadInput
hpc:generated	xsd:anyURI	Generated data, ==hpc:hadOutput
hpc:usedWorkflow	xsd:anyURI	Workflow used
hpc:wasPrecededBy	xsd:anyURI	Experiments before this one
hpc:wasConductedBy	xsd:anyURI	Link to persons
hpc:wasAWS	xsd:anyURI	Software used
hpc:wasAWH	xsd:anyURI	Hardware used
hpc:startDate	xsd:dateTime	Start time
hpc:endDate	xsd:dateTime	End time
hpc:project	xsd:anyURI	Associated projects

D. Artifact and Data

We define Data as a subclass of Artifact and further categorize it into Workflow, Training Dataset, and AI model. We have found that in practice, any combinations of mixed scripts, datasets, and AI model files are shared and reused. They are just vaguely categorized as Data currently. In the HPC software analysis and optimization domain, software itself is also a kind of artifact that can be used as input or output

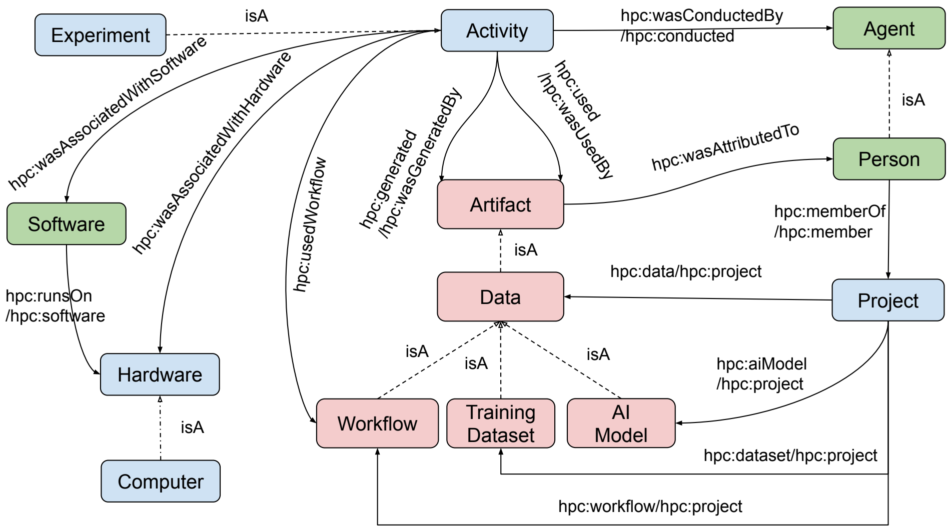
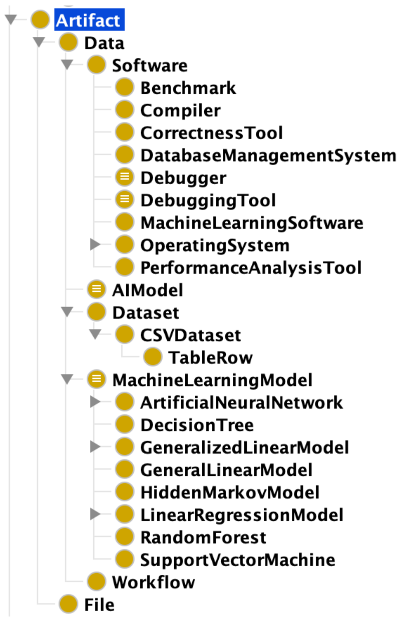


Fig. 2. Major High-level Concepts and Relationships of the HPC Ontology

data. For example, many compilers, tools and workflows process software as input data to generate program analysis information. So there is a property link (*isA*) between Software and Data also. Again, this edge is not shown in Figure 2 to avoid cluttering.

Figure 3 shows the partial class hierarchy rooted at Artifact. *AIModel* is equivalent to *MachineLearningModel* in the figure.



- Artifact
  - Data
    - Software
      - Benchmark
      - Compiler
      - CorrectnessTool
      - DatabaseManagementSystem
      - Debugger
      - DebuggingTool
      - MachineLearningSoftware
      - OperatingSystem
      - PerformanceAnalysisTool
    - AIModel
    - Dataset
      - CSVDataset
        - TableRow
    - MachineLearningModel
      - ArtificialNeuralNetwork
      - DecisionTree
      - GeneralizedLinearModel
      - GeneralLinearModel
      - HiddenMarkovModel
      - LinearRegressionModel
      - RandomForest
      - SupportVectorMachine
    - Workflow
  - File

Fig. 3. Partial class hierarchy of artifact

Table IV shows essential properties for the Data class. There are properties about license, version, associated projects, as well as experiments generating or using the data. Note that Data can be associated with one or more files through the *hpc:file* property. Each file in turn has its properties such as name, size, format, MD5, URL, etc. Data can be derived from other data in a sequence of experiments. So we have *hpc:wasDerivedFrom* to indicate such a property. In the domain of program analysis and optimization, Data generated often has one or more focus applications or machines. We introduce *targetApplication* and *targetMachine* to directly support such links.

TABLE IV
MAJOR PROPERTIES OF THE DATA CLASS

Property	Datatype	Description
hpc:license	xsd:string	License of the data
hpc:version	xsd:string	Version number
hpc:subject	xsd:string	Performance modeling, optimization...
hpc:file	xsd:anyURI	Associated files
hpc:project	xsd:anyURI	Link to the associated projects
hpc:wasGeneratedBy	xsd:anyURI	output of experiments
hpc:wasUsedBy	xsd:anyURI	Input to experiments
hpc:wasDerivedFrom	xsd:anyURI	Some data was derived from other
hpc:targetApplication	xsd:anyURI	Applications being targeted
hpc:targetMachine	xsd:anyURI	Computers being targeted

For Dataset and AI Model classes, they inherit all properties of their superclass Data. They also have additional properties as needed. For example, the AI Model class shown in Table V has extra properties such as source artifacts (*hpc:wasDerivedFromDataset*) used to generate the model, machine learning framework (*hpc:machineLearningFramework*), configurable parameters (*hpc:params*), accuracy (*hpc:accuracy*), and so on. Note that *hpc:wasDerivedFromDataset* (shown in its abbreviation form *hpc:wasDFD*) is a subclass (or a subproperty in ontology's term) of *hpc:wasDerivedFrom*.

E. Software

A piece of software (or a program) can be associated with lots of details. We have to narrow down the scope to

TABLE V
MAJOR PROPERTIES OF THE AI MODEL CLASS

Property	Datatype	Description
hpc:modelFormat	xsd:string	Such as protobuf, onnx, h5
hpc:isTunable	xsd:boolean	Tunable during the runtime or not
hpc:params	xsd:string	Configurable parameters
hpc:framework	xsd:anyURI	Such as TF, PyTorch, MXNet, etc.
hpc:modelType	xsd:string	Relevant problem domains
hpc:supportsAccelerator	xsd:boolean	Run on accelerators or not
hpc:accuracy	xsd:double	Accuracy of the model
hpc:overhead	xsd:double	Overhead of the model
hpc:wasDFD	xsd:string	Datasets used to generate this model
hpc:learningType	xsd:string	Supervised, reinforcement learning, etc.
hpc:learningAlgorithm	xsd:string	Decision tree, random forest, etc.
hpc:hyperParameter	xsd:dict	Hyperparameters such as batch size
hpc:modelProperty	xsd:dict	Such as number and types of layers
hpc:inputShape	xsd:string	Input shape to be fed to the model
hpc:inputDatasetFormat	xsd:string	Input format of the dataset

support generic program analyses and optimizations. In the HPC ontology class hierarchy, Software is a subclass of Data so it has all of Data's properties. We have added a few popular subclasses of Software, including Compiler, OperatingSystem, Benchmark, and so on as shown in Figure 3. In addition, we add the properties shown in Table VI to support brief information about a piece of software or benchmark being analyzed or optimized.

TABLE VI
MAJOR PROPERTIES OF A SOFTWARE PROGRAM/BENCHMARK

Property	Datatype	Description
hpc:programLanguage	xsd:string	Programming languages used
hpc:operatingSystem	xsd:string	OS classes supported
hpc:firstReleaseDate	xsd:date	First release date
hpc:latestReleaseDate	xsd:date	Latest release date
hpc:vendor	xsd:string	Link to vendors
hpc:runsOn	xsd:anyURI	Machines runs the software
hpc:input	xsd:anyURI	Input data of the software
hpc:output	xsd:anyURI	Generated output data

F. Hardware and Computer

The HPC ontology must capture sufficient hardware and computer information to be useful. An HPC computing system can be a single node computer (including a workstation or server) or a cluster with a set of computers. The computer class in the HPC ontology collects the properties describing hardware, performance, and manufacturing related details, as shown in Table VII. Note that some properties should link to structured QUDT data types to encode both values and accurate units. For example, the *hpc:harddriveSize* property has *qudt:QuantityValue* to capture sizes in different units such as GigaBytes or TeraBytes.

We also model CPUs and coprocessors used by a computer. They are linked from a computer object through *hpc:cpu* and *hpc:coprocessor* respectively to provide more information. Table VIII shows some basic CPU class's properties. Given the fast changing nature of CPUs and coprocessors (such as Nvidia GPUs), we model their details in low-level supplemental components with vendor-specific terms and properties. We don't put them into the core, high-level ontology.

TABLE VII
MAJOR PROPERTIES OF THE COMPUTER CLASS

Property	Datatype	Description
hpc:vendor	xsd:string	Vendor of the machine
hpc:cpu	xsd:anyURI	Associated CPUs
hpc:cpuCoresPerNode	xsd:integer	CPU core count
hpc:threadsPerNode	xsd:integer	Threads count
hpc:coprocessor	xsd:anyURI	Associated coprocessors
hpc:coprocessorCoresPerNode	xsd:integer	Coprocessor core count
hpc:memorySize	qudt:QuantityValue	Total memory size
hpc:harddriveSize	qudt:QuantityValue	Total hard drive size
hpc:totalPeakPerformance	qudt:QuantityValue	The peak performance
hpc:hasOperatingSystem	xsd:string	The operating system
hpc:hasCompiler	xsd:string	The compilers available
hpc:power	qudt:QuantityValue	Power consumption
hpc:powerEfficiency	qudt:QuantityValue	Such as GFlops/Watts
hpc:hasRmax	qudt:QuantityValue	Obtained peak perf.
hpc:hasRpeak	qudt:QuantityValue	Theoretical peak
hpc:dateCommissioned	xsd:date	Commission date
hpc:site	xsd:string	Hosting facility/institution
hpc:country	xsd:string	Located country

TABLE VIII
MAJOR PROPERTIES OF THE CPU CLASS

Property	Datatype	Description
hpc:processorTech	xsd:string	Codename/model
hpc:processorGeneration	xsd:string	Processor generation
hpc:processorCorePerSocket	xsd:integer	Cores in a socket
hpc:cpuFrequency	qudt:QuantityValue	Frequency
hpc:memoryBandwidth	qudt:QuantityValue	Memory bandwidth
hpc:processorPeakPerformance	qudt:QuantityValue	Processor performance
hpc:vendor	xsd:string	Link to vendors

Cluster is another class in the HPC ontology, inheriting properties from the Computer subclass, to cover additional properties needed for cluster systems. Each cluster object can be linked to one or more computer objects through its *hasNode* property. Table VII shows major properties of the Cluster class. Given the importance of the Top500 project, a cluster may have related Top500 ranking information (e.g. *hpc:top500Rank*).

TABLE IX
MAJOR PROPERTIES OF THE CLUSTER CLASS

Property	Datatype	Description
hpc:totalClusterCPUCoreCount	xsd:integer	Total CPU cores number
hpc:systemArchitecture	xsd:string	MPP, cluster, etc.)
hpc:computeNodeCount	xsd:integer	Computer node count
hpc:gpuNodeCount	xsd:integer	Number of GPU nodes
hpc:top500Rank	xsd:integer	Top500 ranking
hpc:top500nmax	xsd:integer	Problem size used
hpc:totalCluserMemorySize	qudt:QuantityValue	Total memory
hpc:totalClusterPeakPerformance	qudt:QuantityValue	Total peak performance
hpc:hasNode	xsd:anyURI	Login or compute node

There are a few other high-level concepts such as Person and Project to help describe the semantics of HPC datasets and AI models. We omit their details since their properties are trivial.

V. LOW-LEVEL COMPONENTS OF HPC ONTOLOGY

Low-level components of the HPC Ontology provide fine-granularity concepts and properties to describe subdomains, including hardware details, contents of profiling datasets, and internal details of AI models. They are provided as needed to achieve maximal FAIRness by providing rich attributes to describe data elements. In this paper, we focus on several example subdomains relevant to the scope of our work.

A. A Coprocessor: NVIDIA GPU

For heterogeneous architectures, Nvidia's GPUs are popular components of many supercomputers. Six out of the top ten most powerful computers use Nvidia GPUs, as shown in June 2021's Top500 list [26]. We have added a low-level GPU component into HPC ontology to model the properties of GPUs. Similar low-level components can be added in the future to support other types of heterogeneous processors such as TPU, neuromorphic processors, FPGAs and so on.

Table X shows major properties of a NVIDIA GPU. The properties can be divided into two sets: one is the set of fixed properties of the GPU such as *hpc:theoreticalGPUOccupancy*. The other set includes configurable properties such as *hpc:gpuThreadBlockSize* used to indicate the thread block size configured during a kernel launch.

B. A GPU Performance Dataset: XPlacer

When building AI models for program analyses and optimizations, performance profiling information is often a critical part of the corresponding training datasets. We select a dataset from XPlacer [13] as an example. The dataset contains GPU performance profiling data used to build models guiding GPU memory placement choices for arrays.

A key observation here is that program optimizations often happen at the kernel (or function) level. So we provide properties associated with kernel performance. Table XI lists properties to capture Nvidia GPU's performance profiling information. The properties can be grouped into several categories, including basic information about a kernel and its major data objects (arrays), execution time, and hardware counter based information such as cache utilization rate, page faults, data transfer sizes. Finally, for optimization problems selecting optimal code variants, we provide *hpc:codeVariant* and *hpc:bestCodeVariant* to annotate labels.

VI. Preliminary Results

This section presents some preliminary use cases using the current draft HPC Ontology, including providing standard metadata for annotating various data and answering questions posed as SPARQL queries.

An AWS machine is used to run experiments. It has 4 cores of Intel Xeon CPU E5-2676 v3 running at 2.40GHz and 16 GB main memory. The evaluation uses a set of tools. Protege v5.5.0 is used for ontology development. Typically raw data is stored in CSV files. Tarql (git hash #b06b4dd) [27] is used to automatically convert CSV files into RDF triples saved into N-Triples (.NT) files. Tarql's conversion rules are manually specified using SPARQL 1.1 syntax. Blazegraph v2.1.6 is used as the graph database supporting standard RDF/SPARQL APIs. All N-Triples files are loaded into a namespace of Blazegraph in a triples mode and inference turned on.

JSON-LD, a JSON-based format storing Linked Data, is used as the main format to present annotated data. JSON-LD can be viewed as JSON plus Context and ID information. The context is used to define the short-hand names. IDs are unique name identifiers to describe keys in the document. These IDs are used as the keys of JSON's key-value pairs to unambiguously encoding information linked to formally defined entities in an ontology. We use a Python script calling RDFLib APIs to generate the JSON-LD output from .NT files.

A. Providing Metadata for Top500 Supercomputers

Machine properties are fundamental information in HPC. We use the concepts and properties of the HPC ontology to annotate the tabular information of the fastest machine, Supercomputer Fugaku, published in June 2021's Top500 list [26].

The HPC Ontology has all the concepts and properties needed to fully annotate the content of the entire top 500 spreadsheet. Listing 2 shows various example properties of Fugaku in JSON-LD format. All properties are stored in key-value pairs. The machine is uniquely identified by its system ID (179807) assigned by the Top500 website. The HPC ontology provides vocabularies of property names, such as *hpc:name*, *hpc:Cluster*, and *hpc:power*. The QUDT ontology provides structured values with detailed information for the units used, such as MegaHZ and KiloWatt. Note that QUDT originally did not have the TeraFLOPS unit; we have extended it to support this.

Listing 2. Example Fugaku's Information Annotated Using HPC Ontology

```
{
  "@id": "https://www.top500.org/system/179807",
  "@type": "hpc:Cluster",
  "hpc:name": "Supercomputer Fugaku",
  "hpc:top500Rank": 1,
  "hpc:vendor": "Fujitsu",
  "hpc:country": "Japan",
  "hpc:cpuArchitecture":"Fujitsu ARM",
  "hpc:cpuFrequency": { "@id": "_:B9e8a3"  },
  "hpc:hasOperatingSystem": "Red Hat Enterprise Linux",
  "hpc:hasRmax": {  "@id": "_:B17f29"  },
  "hpc:power": { "@id": "_:N15c5a" },
  "hpc:processorCorePerSocket": 48,
  "hpc:processorGeneration": "Fujitsu A64FX",
  "hpc:site": "RIKEN Center for Computational Science",
  "hpc:systemArchitecture": "MPP",
  "hpc:systemModel": "Supercomputer Fugaku",
  "hpc:totalClusterCPUCoreCount": 7630848
},

{ "@id": "_:B17f29",
  "@type": "qudt:QuantityValue",
  "qudt:unit": { "@id": "http://qudt.org/vocab/unit/
     TeraFLOPS"},
  "qudt:value": "442010.00"
},

{ "@id": "_:B9e8a3",
  "@type": "qudt:QuantityValue",
  "qudt:unit": {"@id": "http://qudt.org/vocab/unit/MegaHZ
     "},
  "qudt:value": "2200"
},

{ "@id": "_:N15c5a",
  "@type": "qudt:QuantityValue",
```

TABLE X
MAJOR PROPERTIES OF A NVIDIA GPU

Property	Datatype	Description
hpc:dramFrequency	qudt:QuantityValue	Frequency of DRAM
hpc:streamingMultiprocessorFrequency	qudt:QuantityValue	Frequency of Streaming multiprocessor
hpc:activeCyclesOfStreamingMultiprocessor	xsd:integer	Active cycle counts from SM
hpc:theoreticalActiveWarpsPerSM	xsd:integer	Theoretical Active Warps per SM
hpc:theoreticalGPUOccupancy	xsd:double	Theoretical Occupancy
hpc:maxGPUThreadBlockSizeLimitedBySM	xsd:integer	Max block limited by SM
hpc:maxGPUThreadBlockSizeLimitedByRegister	xsd:integer	Max block limited by registers
hpc:maxGPUThreadBlockSizeLimitedBySharedMemory	xsd:integer	Max block limited by shared memory
hpc:maxGPUThreadBlockSizeLimitedByWarps	xsd:integer	Max block limited by warps
hpc:gpuThreadBlockSize	xsd:integer	Launch block size
hpc:gpuThreadGridSize	xsd:integer	Launch grid size
hpc:registersPerThread	xsd:integer	Launch register//thread
hpc:gpuSharedMemoryConfigurationSize	qudt:QuantityValue	Launch shared memory configuration size
hpc:gpuStaticSharedMemorySizePerBlock	qudt:QuantityValue	launch static shared memory
hpc:gpuThreadCount	xsd:integer	GPU thread count
hpc:gpuWavesPerSM	xsd:integer	Launch wave per SM
hpc:gpuUnifiedMemoryRemoteMapSize	qudt:QuantityValue	Unified memory remote map

TABLE XI
MAJOR PROPERTIES OF KERNEL PERFORMANCE PROFILING DATA

Property	Datatype	Description
Kernel Information		
hpc:kenelName	xsd:string	Kernel/function name
hpc:benchmark	xsd:anyURI	Associated benchmark
hpc:commandLineOption	xsd:string	Command line Options
hpc:arrayName	xsd:string	Name of array
hpc:allocatedDataSize	qudt:QuantityValue	Memory allocation size
hpc:beginMemoryAddress	xsd:string	Beginning array address
hpc:endMemoryAddress	xsd:string	Ending array address
Performance Information		
hpc:cycle	xsd:integer	Profiled cycle count
hpc:executionTime	qudt:QuantityValue	Execution time
hpc:numberOfCalls	xsd:integer	Number of calls
hpc:averageExecutionTime	qudt:QuantityValue	Average execution time
hpc:minExecutionTime	qudt:QuantityValue	Min. execution time
hpc:maxExecutionTime	qudt:QuantityValue	Max. execution time
hpc:executionTimePercentage	xsd:double	Percentage of time spent
hpc:memoryThroughputRate	xsd:double	Memory Throughput
hpc:dramUtilizationRate	xsd:double	DRAM utilization rate
hpc:l1CacheUtilizationRate	xsd:double	L1/Tex utilization rate
hpc:l2CacheUtilizationRate	xsd:double	L2 utilization rate
hpc:achievedGPUOccupancy	xsd:double	GPU occupancy
hpc:achievedActiveWarpsPerSM	xsd:integer	Active warps per SM
hpc:cpuPageFault	xsd:integer	CPU page fault count
hpc:gpuPageFault	xsd:integer	GPU page fault count
hpc:hostToDeviceTransferSize	qudt:QuantityValue	HostToDevice transfer
hpc:deviceToHostTransferSize	qudt:QuantityValue	DeviceToHost transfer
Labels		
hpc:codeVariant	xsd:integer	Code variant ID
hpc:labeledCodeVariant	xsd:integer	Best variant ID

```
  "qudt:unit": {"@id": "http://qudt.org/vocab/unit/KiloW"},
  "qudt:value": "29899.23"
}
```

B. Providing Metadata for Datasets and AI Models

We are developing a web portal to allow users to submit information about training datasets and AI models in HPC. To make the submitted data complaint with the FAIR principals, standard metadata must be used to annotate the datasets and AI models. The HPC ontology can serve as the metadata for this purpose.

Listing 3 shows a benchmark software package [28] which was used as an input dataset for a code similarity analysis experiment. It is easy to identify metadata for its name, license, subject, related project, and so on.

Listing 3. Example Dataset Annotated Using HPC Ontology

```
{
  "@id": "http://example.org/dataset/DA000005",
  "@type": "hpc:Dataset",
  "hpc:description": "microbenchmark kernels in C/C++ and
     Fortran",
  "hpc:hasIDType": "System Generated",
  "hpc:license": "BSD",
  "hpc:name": "DataRaceBench micro-benchmarks",
  "hpc:project": {
    "@id": "http://example.org/project/PR000002"
  },
  "hpc:subject": [
    "OpenMP",
    "Data Race Detection",
    "Computer Science"
  ],
  "hpc:url": "https://github.com/LLNL/dataracebench/tree/
     master/micro-benchmarks",
  "hpc:version": "1.3.2"
}
```

Listing 4 shows metadata for an AI model released by a study [13]. Besides common metadata for its name and type, it additionally has metadata specific to this AI model, such as *hpc:wasDerivedFromDataset*, *hpc:learningAlgorithm*, and *hpc:targetMachine*.

Listing 4. Example AI model annotated using HPC ontology

```
{
  "@id": "http://example.org/AIModel/MO000001",
  "@type": "hpc:AIModel",
  "hpc:contributor":
    {"@id": "http://example.org/person/PI000013"  },
  "hpc:description": "Onnx version of the decision tree
     model for XPlacer",
  "hpc:wasGeneratedBy":
     {"@id": "http://example.org/experiment/EX000002"},
  "hpc:hasIDType": "System Generated",
  "hpc:wasDerivedFromDataset": [
    {"@id": "http://example.org/dataset/DA000001"},
    {"@id": "http://example.org/dataset/DA000002"},
    {"@id": "http://example.org/dataset/DA000003"},
    {"@id": "http://example.org/dataset/DA000004"}
  ],
  "hpc:isTunable": false,
  "hpc:learningType": "Supervised ",
  "hpc:modelFormat": "ONNX",
  "hpc:modelType": "Prediction",
  "hpc:learningAlgorithm" : "Decision Tree",
  "hpc:name": "decisionTree.onnx",
  "hpc:project":
       {"@id":"http://example.org/project/PR000001"},
  "hpc:subject": [
    "GPGPU",
    "Heterogeneous Systems",
    "Data Placement",
    "Decision Tree"
  ],
  "hpc:supportsAccelerator": true,
  "hpc:targetMachine":
      {"@id": "http://example.org/cluster/lassen"},
  "hpc:url": "https://github.com/xyz/decisionTree.onnx"
  },
  "hpc:version": "1.2.1"
}
```

C. Encoding GPU Profiling Dataset Stored in a CSV File

Low-level components of the HPC ontology can be used to encode the internal content of datasets or AI models. Listing 5 shows the annotation of a row of a CSV file representing a dataset released by a study [13]. Each row represents information about an array accessed within a kernel code variant and the kernel's associated profiling metrics such as GPU data transferring data sizes and page faults. The dataset was used to train a model deciding which code variant delivers the best performance. Using properties defined in Table XI, the annotated json-ld file contains accurate, machine readable information for each cell, which facilitates interoperability and reusability of the dataset.

Listing 5. Example profiling dataset annotated using HPC ontology

```
{
  "@id": "https://github.com/xyz/rodinia_3.1
     _cuda_bfs_datalevel-lassen.csv#L11",
  "@type": "hpc:TableRow",
  "hpc:BeginMemoryAddress": "0x200060080000",
  "hpc:EndMemoryAddress": "0x200060090000",
  "hpc:allocatedDataSize": 65536,
  "hpc:arrayID": "1",
  "hpc:arrayName": "h_graph_mask",
  "hpc:codeVariant": "111100",
  "hpc:commandLineOption": "graph65536",
  "hpc:cpuPageFault": 2,
      "hpc:deviceToHostTransferSize": {
        "@id": "_:Nca485"
      },
      "hpc:hostToDeviceTransferSize": {
        "@id": "_:Na7702" }
    },
  {
   "@id": "_:Na7702",
   "@type": "qudt:QuantityValue",
   "qudt:unit": {
     "@id": "http://qudt.org/vocab/unit/KiloBYTE"   },
   "qudt:value": {
     "@type": "http://www.w3.org/2001/XMLSchema#decimal",
     "@value": "192.0"   }
  },
  {
    "@id": "_:Nca485",
    "@type": "qudt:QuantityValue",
      "qudt:unit": {
        "@id": "http://qudt.org/vocab/unit/KiloBYTE"
      },
   "qudt:value": {
     "@type": "http://www.w3.org/2001/XMLSchema#decimal",
     "@value": "0.0"
   }
  }
```

D. Enabling Various Queries

A standard approach to evaluating an ontology is to check if the ontology can be used to formulate questions asked by intended users. Such questions often are called competency questions. We anticipate some typical questions from a HPC user may include the following:

- Q1: What are the ids of datasets from a research project named "Xplacer"?
- Q2: What are the names of AI models available for a supercomputer named "lassen"?
- Q3: What AI models are available for machines with GPUs named "Nvidia V100"?
- Q4: What datasets of projects funded by NSF are available for building Performance Prediction models?
- Q5: What workflows are available for generating AI models guiding "Heterogeneous Mapping" of a benchmark (e.g. the NAS Parallel Benchmark or NPB) running on a machine using AMD GPUs?

We populated a Blazegraph RDF database with information encoding a few example datasets and AI models found in the literature, assuring diversified datasets and models across widely researched domains. We gathered data from projects like XPlacer [13] that come with the workflows defining dataset collection and offer models to perform experiments. Further, there were scenarios when researchers publish their results as a package or complete tool. The ProGraML [29] and MLGO [30] are such considered examples. Additionally, we included literature from HPC Energy Research [31] providing datasets or models alone. We also collected some datasets and refined models hosted at Kaggle. They are related to the GPU Kernel Performance [32]–[34].

Listing 6 shows the SPARQL queries sent to the Blazegraph database and the corresponding answers obtained, for Q1 through Q3. Listing 7 shows queries and results for Q3 and Q4. The results show that HPC Ontology is complete to support the concepts and properties expressed in these queries which in turn obtain desired results.

Listing 6. SPARQL queries to answer competency questions 1-3

```
PREFIX hpc: <https://example.org/HPC-Ontology#>
# Query for Q1: dataset ids of a project
#------------------------------------------------------
SELECT ?ds
WHERE { ?pid rdf:type hpc:Project .
        ?pid hpc:name "Xplacer" .
        ?pid hpc:dataset ?ds }

# Results: IDs of datasets
# <http://example.org/dataset/DA000001>
# <http://example.org/dataset/DA000002>
# <http://example.org/dataset/DA000003>
# <http://example.org/dataset/DA000004>

# Query for Q2: AI models' names of a supercomputer
#------------------------------------------------------
SELECT ?model_name
WHERE { ?model_id rdf:type hpc:AIModel .
        ?model_id hpc:targetMachine
            <http://example.org/cluster/lassen> .
        ?model_id hpc:name ?model_name }

# Results : names of AI models
# decisionTree.onnx
# randomForest.onnx

# Query for Q3: machines with NVidia V100 and their models
#---------------------------------------------------------
SELECT ?machine ?model_id
  WHERE { ?gpu rdf:type hpc:GPU .
          ?gpu hpc:name "Nvidia V100".
            ?machine hpc:coprocessorModel ?gpu .
            ?model_id hpc:targetMachine ?machine .
            ?model_id rdf:type hpc:AIModel .
            ?model_id hpc:name ?model_name  }

# Results: machine names and AI model IDs
<http://example.org/cluster/lassen> <http://example.org/
     AIModel/MO000001>
<http://example.org/cluster/lassen> <http://example.org/
     AIModel/MO000002>
```

Listing 7. SPARQL queries to answer competency questions 4-5

```
PREFIX hpc: <https://example.org/HPC-Ontology#>

# Query for Q4: NSF project's datasets for building
     performance prediction models
#---------------------------------------------------------
SELECT ?project_id ?ds_id
WHERE {
        ?project_id rdf:type hpc:Project .
        ?project_id hpc:fundedBy "the National Science
     Foundation" .
        ?ds_id hpc:project ?project_id .
        ?ds_id rdf:type hpc:Dataset .
        ?ds_id hpc:subject "Performance Prediction" }

# Results: project IDs and dataset IDs
<http://example.org/project/PR000003> <http://example.org/
     dataset/DA000007>
<http://example.org/project/PR000003> <http://example.org/
     dataset/DA000008>
<http://example.org/project/PR000003> <http://example.org/
     dataset/DA000009>

# Query of Q5: workflow generating AI models for NPB's
     heterogeneous mapping on AMD GPU
SELECT ?pid ?pname
WHERE {
        ?pid rdf:type hpc:Workflow .
        ?pid hpc:subject "Heterogeneous Mapping" .
        ?pid hpc:name ?pname .

        ?pid hpc:targetMachine ?machine_id .
        ?machine_id hpc:coProcessor ?gpu_id .
        ?gpu_id hpc:vendor "AMD" .

        ?pid hpc:targetApplication ?app_id .
        ?app_id hpc:name "NPB" .
      }

# Results
<http://example.org/workflow/WF000020>  OpenCL
     Heterogeneous Mapping
```

VII. Related Work

Due to their consistency and expressivity, numerous ontologies [35]–[38] have been developed to effectively combine data or information from multiple heterogeneous sources. For example, DBpedia [25], [39] extracts entities and relations from Wikipedia to create an ontology which becomes a natural hub for connecting datasets. Sun et al. [40] developed Geospatial data ontology as the semantic foundation of geospatial data integration and sharing. Their ontology is a framework with three dimensions. The ontological category dimension has general, domain, and application-level ontologies. The content dimension has essential, morphology, and provenance ontologies. Finally, the logic dimension has classes, relations, properties, and instances. Google, Bing and Yahoo rely on schema.org [21], essentially a public shared ontology, to maintain a list of vocabularies that developers can use to publish structured data about web pages. This ontology also drives features like Google's Knowledge Graph. Brick [23], [41] is a domain-specific ontology to enable portable applications managing commercial buildings.

Ontologies have been studied to improve machine learning in various aspects, including sentiment classification, answer evaluation, personalized recommendation and so on [42]. OntoDM [43] is an ontology of data mining. Sudathip et al. [44] presented a machine learning ontology covering concepts from learning, applications, techniques, and evaluation. Xu et al. proposed an OWL ontology to make machine-learned functions findable on the web [45]. VIS4ML [46] is an ontology for visual analytics assisted machine learning. It can be used to describe ML workflows. Hwang et al. proposed a task ontology to enable autonomous machine learning modeling [47].

Some studies leveraged ontologies For program analyses and optimizations. Yue et al. developed ontology-based program analysis [48]. Liao et al. explored ontologies to enhance domain-specific language implementations [49]. Pattipati et al. [50] built an extensible framework for ontology-based advanced program analysis.

VIII. Conclusion

This paper presents our ongoing efforts to build an ontology to enable FAIR datasets and AI models in the HPC program analysis and optimization domain. We adopt a two-level design to be lightweight and extensible. The resulting HPC Ontology has modeled properties of essential concepts in the domain, including computers, experiments, software, hardware, datasets, AI models, and so on. Preliminary results show that our design is effective to annotate both high-level metadata and low-level details of selected sample data. The ontology is also able to support typical competency questions formed as SPARQL queries.

Future work will include more low-level supplement components. Examples include more comprehensive AI model categories and properties describing internal details of different machine learning models. We will also add a workflow component in order to support workflow synthesizing in HPC. Automated techniques will be explored for generating RDF triples describing more software, hardware, HPC datasets and AI models. The current draft HPC Ontology is available online [1] under a Creative Commons license to collect community input. We welcome community comments and suggestions to enhance the ontology.

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[1]https://hpc-fair.github.io/ontology/

References

[1] P. Malakar, P. Balaprakash, V. Vishwanath, V. Morozov, and K. Kumaran, "Benchmarking machine learning methods for performance modeling of scientific applications," in *2018 IEEE/ACM Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS)*. IEEE, 2018, pp. 33–44.

[2] J. Sun, S. Zhan, G. Sun, and Y. Chen, "Automated performance modeling based on runtime feature detection and machine learning," in *2017 IEEE International Symposium on Parallel and Distributed Processing with Applications and 2017 IEEE International Conference on Ubiquitous Computing and Communications (ISPA/IUCC)*. IEEE, 2017, pp. 744–751.

[3] K. Singh, E. İpek, S. A. McKee, B. R. de Supinski, M. Schulz, and R. Caruana, "Predicting parallel application performance via machine learning approaches," *Concurrency and Computation: Practice and Experience*, vol. 19, no. 17, pp. 2219–2235, 2007.

[4] U. Lopez-Novoa, A. Mendiburu, and J. Miguel-Alonso, "A survey of performance modeling and simulation techniques for accelerator-based computing," *IEEE Transactions on Parallel and Distributed Systems*, vol. 26, no. 1, pp. 272–281, 2014.

[5] T. Islam, A. Ayala, Q. Jensen, and K. Ibrahim, "Toward a programmable analysis and visualization framework for interactive performance analytics," in *2019 IEEE/ACM International Workshop on Programming and Performance Visualization Tools (ProTools)*. IEEE, 2019, pp. 70–77.

[6] J. J. Thiagarajan, R. Anirudh, B. Kailkhura, N. Jain, T. Islam, A. Bhatele, J.-S. Yeom, and T. Gamblin, "Paddle: Performance analysis using a data-driven learning environment," in *2018 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, 2018, pp. 784–793.

[7] O. Tuncer, E. Ates, Y. Zhang, A. Turk, J. Brandt, V. J. Leung, M. Egele, and A. K. Coskun, "Diagnosing performance variations in hpc applications using machine learning," in *International Supercomputing Conference*. Springer, 2017, pp. 355–373.

[8] S. Jayasena, S. Amarasinghe, A. Abeyweera, G. Amarasinghe, H. De Silva, S. Rathnayake, X. Meng, and Y. Liu, "Detection of false sharing using machine learning," in *Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis*, 2013, pp. 1–9.

[9] J. Vetter, "Performance analysis of distributed applications using automatic classification of communication inefficiencies," in *Proceedings of the 14th international conference on Supercomputing*, 2000, pp. 245–254.

[10] A. Borghesi, A. Bartolini, M. Lombardi, M. Milano, and L. Benini, "Anomaly detection using autoencoders in high performance computing systems," in *Proceedings of the AAAI Conference on Artificial Intelligence*, vol. 33, 2019, pp. 9428–9433.

[11] A. Das, F. Mueller, P. Hargrove, E. Roman, and S. Baden, "Doomsday: predicting which node will fail when on supercomputers," in *SC18: International Conference for High Performance Computing, Networking, Storage and Analysis*. IEEE, 2018, pp. 108–121.

[12] Y. Zhao, J. Li, C. Liao, and X. Shen, "Bridging the gap between deep learning and sparse matrix format selection," in *Proceedings of the 23rd ACM SIGPLAN symposium on principles and practice of parallel programming*, 2018, pp. 94–108.

[13] H. Xu, M. Emani, P.-H. Lin, L. Hu, and C. Liao, "Machine learning guided optimal use of gpu unified memory," in *2019 IEEE/ACM Workshop on Memory Centric High Performance Computing (MCHPC)*. IEEE, 2019, pp. 64–70.

[14] N. Sukhija, B. Malone, S. Srivastava, I. Banicescu, and F. M. Ciorba, "A learning-based selection for portfolio scheduling of scientific applications on heterogeneous computing systems," *Parallel and Cloud Computing*, vol. 3, no. 4, pp. 66–81, 2014.

[15] K. Fagnan, Y. Nashed, G. Perdue, D. Ratner, A. Shankar, and S. Yoo, "Data and models: a framework for advancing ai in science," USDOE Office of Science (SC)(United States), Tech. Rep., 2019.

[16] M. D. Wilkinson, M. Dumontier, I. J. Aalbersberg, G. Appleton, M. Axton, A. Baak, N. Blomberg, J.-W. Boiten, L. B. da Silva Santos, P. E. Bourne *et al.*, "The fair guiding principles for scientific data management and stewardship," *Scientific data*, vol. 3, no. 1, pp. 1–9, 2016.

[17] B. Motik, P. F. Patel-Schneider, B. Parsia, C. Bock, A. Fokoue, P. Haase, R. Hoekstra, I. Horrocks, A. Ruttenberg, U. Sattler *et al.*, "Owl 2 web ontology language: Structural specification and functional-style syntax," *W3C recommendation*, vol. 27, no. 65, p. 159, 2009.

[18] M. Uschold and M. Gruninger, "Ontologies: Principles, methods and applications," *The knowledge engineering review*, vol. 11, no. 2, pp. 93–136, 1996.

[19] S. Staab and R. Studer, *Handbook on ontologies*. Springer Science & Business Media, 2013.

[20] J. Ison, M. Kalaš, I. Jonassen, D. Bolser, M. Uludag, H. McWilliam, J. Malone, R. Lopez, S. Pettifer, and P. Rice, "Edam: an ontology of bioinformatics operations, types of data and identifiers, topics and formats," *Bioinformatics*, vol. 29, no. 10, pp. 1325–1332, 2013.

[21] R. V. Guha, D. Brickley, and S. Macbeth, "Schema.org: evolution of structured data on the web," *Communications of the ACM*, vol. 59, no. 2, pp. 44–51, 2016.

[22] M. A. Jensen, V. Ferretti, R. L. Grossman, and L. M. Staudt, "The nci genomic data commons as an engine for precision medicine," *Blood*, vol. 130, no. 4, pp. 453–459, 2017.

[23] B. Balaji, A. Bhattacharya, G. Fierro, J. Gao, J. Gluck, D. Hong, A. Johansen, J. Koh, J. Ploennigs, Y. Agarwal *et al.*, "Brick: Metadata schema for portable smart building applications," *Applied energy*, vol. 226, pp. 1273–1292, 2018.

[24] S. L. Weibel and T. Koch, "The dublin core metadata initiative," *D-lib magazine*, vol. 6, no. 12, pp. 1082–9873, 2000.

[25] P. N. Mendes, M. Jakob, and C. Bizer, "Dbpedia: A multilingual cross-domain knowledge base." in *LREC*. Citeseer, 2012, pp. 1813–1817.

[26] "Top500 List, June 2021," https://www.top500.org/lists/top500/2021/06/, June, 2021.

[27] "Sparql for tables: Turn csv into rdf using sparql syntax," https://tarql.github.io/, accessed: 2021-06-09.

[28] C. Liao, P.-H. Lin, J. Asplund, M. Schordan, and I. Karlin, "Dataracebench: a benchmark suite for systematic evaluation of data race detection tools," in *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, 2017, pp. 1–14.

[29] C. Cummins, Z. Fisches, T. Ben-Nun, T. Hoefler, M. O'Boyle, and H. Leather, "ProGraML: A Graph-based Program Representation for Data Flow Analysis and Compiler Optimizations," in *Thirty-eighth International Conference on Machine Learning (ICML)*, 2021.

[30] M. Trofin, Y. Qian, E. Brevdo, Z. Lin, K. Choromanski, and D. Li, "Mlgo: a machine learning guided compiler optimizations framework," *arXiv preprint arXiv:2101.04808*, 2021.

[31] C. Phillipsy, "Hpc energy research," 2016. [Online]. Available: https://cscdata.nrel.gov/#/datasets/d332818f-ef57-4189-ba1d-beea291886eb"

[32] R. Ballester-Ripoll, E. G. Paredes, and R. Pajarola, "Sobol tensor trains for global sensitivity analysis," *Reliability Engineering & System Safety*, vol. 183, pp. 311–322, 2019.

[33] C. Nugteren and V. Codreanu, "Cltune: A generic auto-tuner for opencl kernels," in *2015 IEEE 9th International Symposium on Embedded Multicore/Many-core Systems-on-Chip*. IEEE, 2015, pp. 195–202.

[34] R. Shrivastava, "Gpu kernel performance dataset," https://www.kaggle.com, 2020.

[35] F. M. Suchanek, G. Kasneci, and G. Weikum, "Yago: A large ontology from wikipedia and wordnet," *Journal of Web Semantics*, vol. 6, no. 3, pp. 203–217, 2008.

[36] C. Matuszek, J. Cabral, M. J. Witbrock, and J. DeOliveira, "An introduction to the syntax and content of cyc." in *AAAI Spring Symposium: Formalizing and Compiling Background Knowledge and Its Applications to Knowledge Representation and Question Answering*. Citeseer, 2006, pp. 44–49.

[37] M. A. Sicilia, E. Garcia, S. Sanchez, and E. Rodriguez, "On integrating learning object metadata inside the opencyc knowledge base," in *IEEE International Conference on Advanced Learning Technologies, 2004. Proceedings.* IEEE, 2004, pp. 900–901.

[38] A. Pease, I. Niles, and J. Li, "The suggested upper merged ontology: A large ontology for the semantic web and its applications," in *Working notes of the AAAI-2002 workshop on ontologies and the semantic web*, vol. 28, 2002.

[39] S. Auer, C. Bizer, G. Kobilarov, J. Lehmann, R. Cyganiak, and Z. Ives, "Dbpedia: A nucleus for a web of open data," in *The semantic web*. Springer, 2007, pp. 722–735.

[40] K. Sun, Y. Zhu, P. Pan, Z. Hou, D. Wang, W. Li, and J. Song, "Geospatial data ontology: the semantic foundation of geospatial data integration and sharing," *Big Earth Data*, vol. 3, no. 3, pp. 269–296, 2019.

[41] B. Balaji, A. Bhattacharya, G. Fierro, J. Gao, J. Gluck, D. Hong, A. Johansen, J. Koh, J. Ploennigs, Y. Agarwal *et al.*, "Brick: Towards a unified metadata schema for buildings," in *Proceedings of the 3rd*

ACM International Conference on Systems for Energy-Efficient Built Environments, 2016, pp. 41–50.

[42] L. Rachana and S. Shridevi, "A literature survey: semantic technology approach in machine learning," *Advances in Smart Grid Technology*, pp. 467–477, 2021.

[43] P. Panov, S. Džeroski, and L. Soldatova, "Ontodm: An ontology of data mining," in *2008 IEEE International Conference on Data Mining Workshops*. IEEE, 2008, pp. 752–760.

[44] K. Sudathip and M. Sodanil, "Ontology knowledge-based framework for machine learning concept," in *Proceedings of the 18th International Conference on Information Integration and Web-based Applications and Services*, 2016, pp. 50–53.

[45] J. Xu, H. Wang, and H. Trimbach, "An owl ontology representation for machine-learned functions using linked data," in *2016 IEEE International Congress on Big Data (BigData Congress)*. IEEE, 2016, pp. 319–322.

[46] D. Sacha, M. Kraus, D. A. Keim, and M. Chen, "Vis4ml: An ontology for visual analytics assisted machine learning," *IEEE transactions on visualization and computer graphics*, vol. 25, no. 1, pp. 385–395, 2018.

[47] K. S. Hwang, K. S. Park, S. H. Lee, K. I. Kim, and K. M. Lee, "Autonomous machine learning modeling using a task ontology," in *2018 Joint 10th International Conference on Soft Computing and Intelligent Systems (SCIS) and 19th International Symposium on Advanced Intelligent Systems (ISIS)*. IEEE, 2018, pp. 244–248.

[48] Y. Zhao, G. Chen, C. Liao, and X. Shen, "Towards ontology-based program analysis," in *30th European Conference on Object-Oriented Programming (ECOOP 2016)*. Schloss Dagstuhl-Leibniz-Zentrum fuer Informatik, 2016.

[49] C. Liao, P.-H. Lin, D. J. Quinlan, Y. Zhao, and X. Shen, "Enhancing domain specific language implementations through ontology," in *Proceedings of the 5th International Workshop on Domain-Specific Languages and High-Level Frameworks for High Performance Computing*, 2015, pp. 1–9.

[50] D. K. Pattipati, R. Nasre, and S. K. Puligundla, "Opal: An extensible framework for ontology-based program analysis," *Software: Practice and Experience*, vol. 50, no. 8, pp. 1425–1462, 2020.