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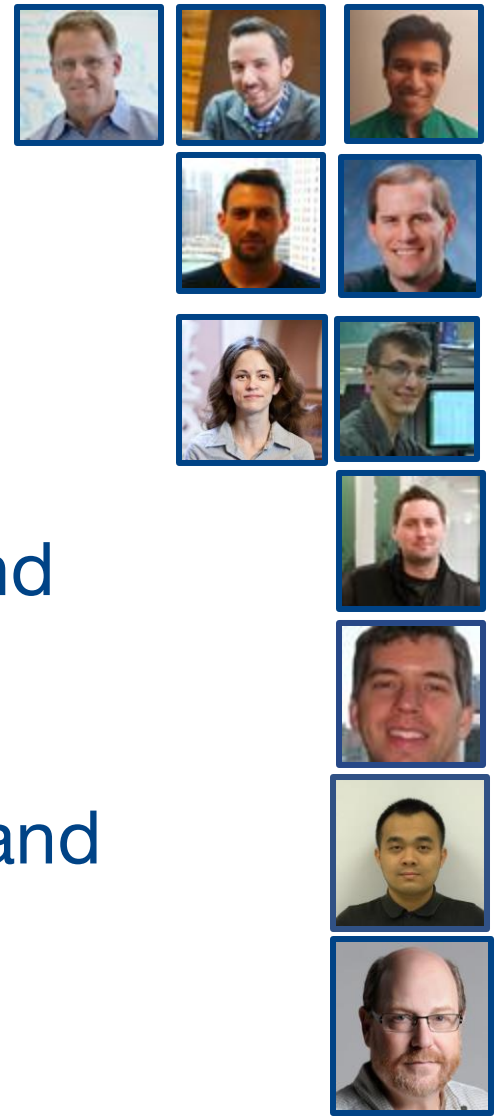
DLHub

Data and Learning Hub for Science

Ben Blaiszik (bblaiszik@anl.gov), Ryan Chard, Logan Ward,
Kyle Chard, Zhuozhao Li, Anna Woodard, Yadu Babuji,
Steve Tuecke, Mike Franklin, Ian Foster

Funding: 2018 Argonne Advanced Computing LDRD

Data and Learning Hub for Science (DLHub)



- Collect, publish, categorize models from many disciplines (materials science, physics, chemistry, genomics, etc.)
- Serve models via API to simplify sharing, consumption, and access
- Enable new science through reuse, real-time integration, and synthesis of existing models

Funding: 2018 Argonne Adv. Computing LDRD

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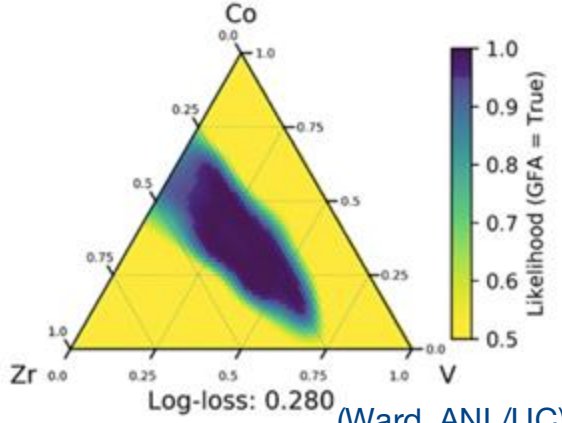
Select DLHub Use Cases

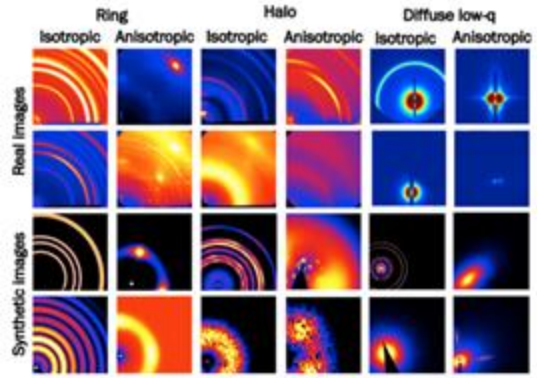
Model-driven Experimentation and Data Tagging

- Metallic glass discovery [active learning]



(Ward, ANL/UC)

- XRD beamline image tagging

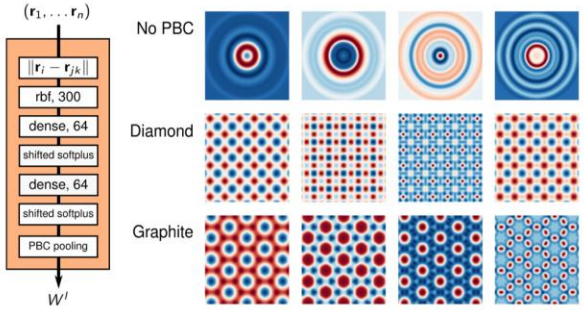


	probability	tags
1	0.999780	Beam Off Image
6	0.745707	Halo
13	0.364863	Strong scattering
7	0.082574	High background
12	0.027826	Ring
8	0.012137	Higher orders
15	0.008106	Weak scattering
9	0.001964	Linear beamstop
16	0.001744	Wedge beamstop
2	0.000982	Circular Beamstop

(Yager, BNL)

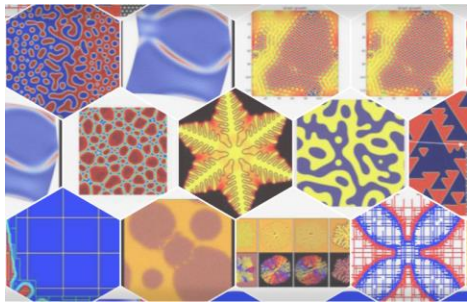
Community Model Benchmarking

- Crystal structure



(Ward, ANL/UC)

- NIST PFHub



(Wheeler, Warren, Heinonen NIST/UC/Argonne/NU)

Automated Model Retraining with New Data

- Models linked to dynamic data sources

(Center for Hierarchical Materials Design NIST/UC/Argonne/NU)

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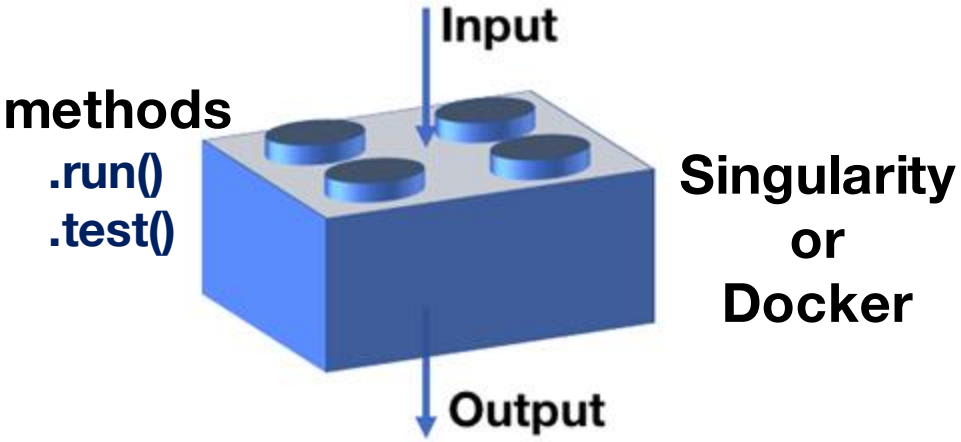
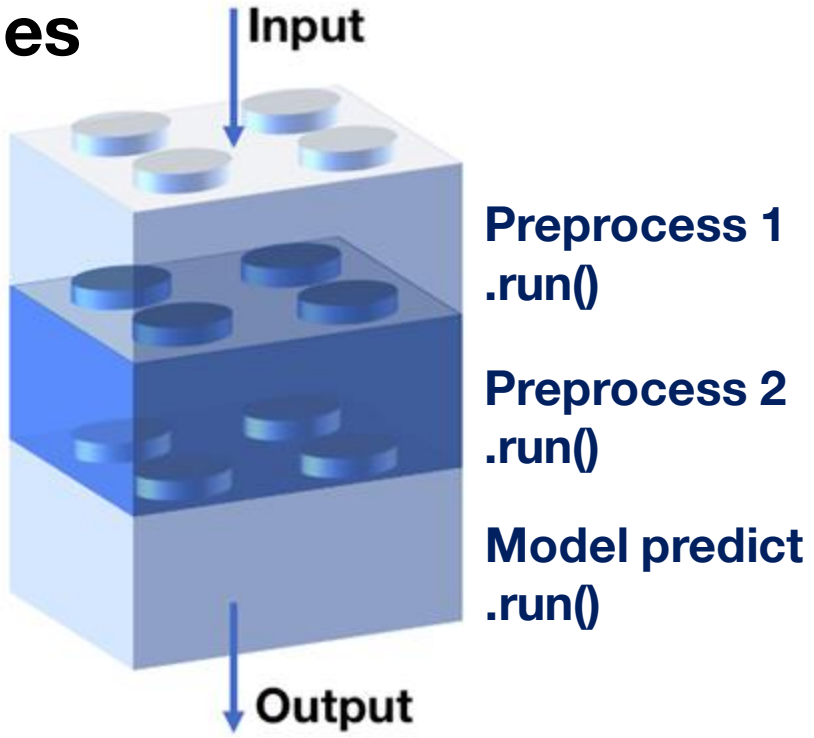
DLHub Servables and Pipelines

Servables



Pipelines



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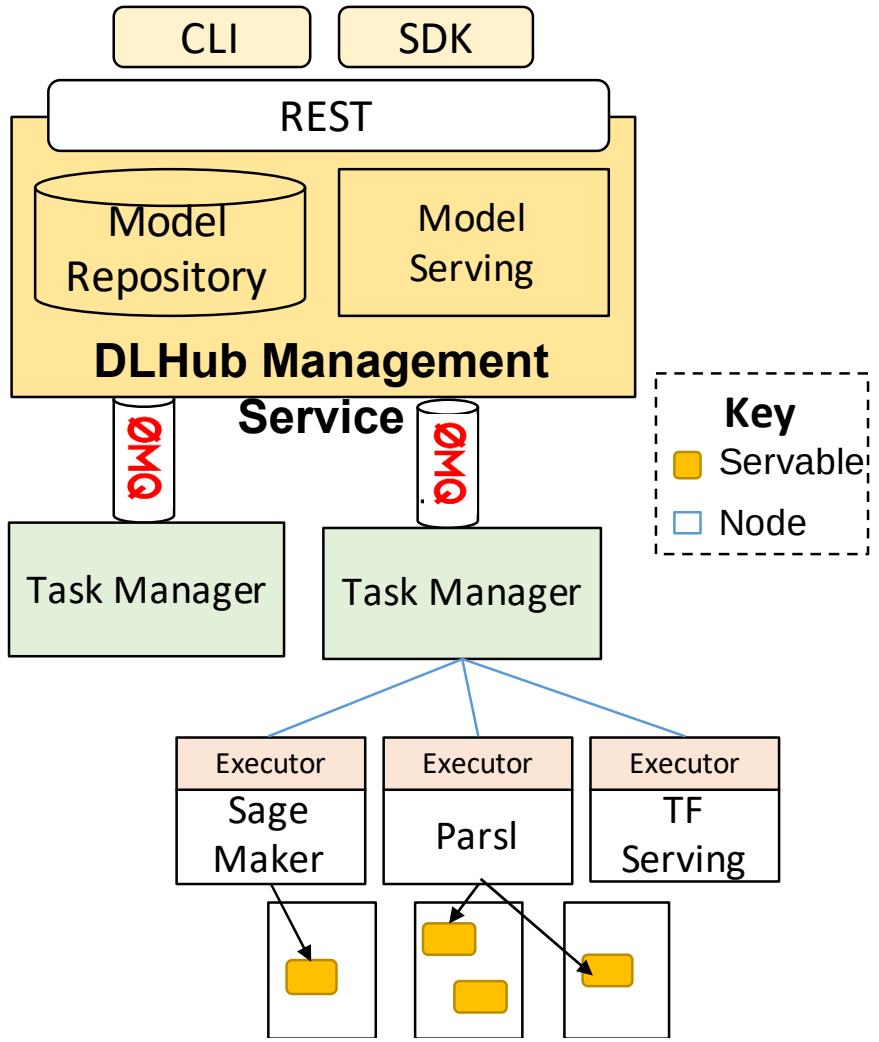
DLHub Architecture

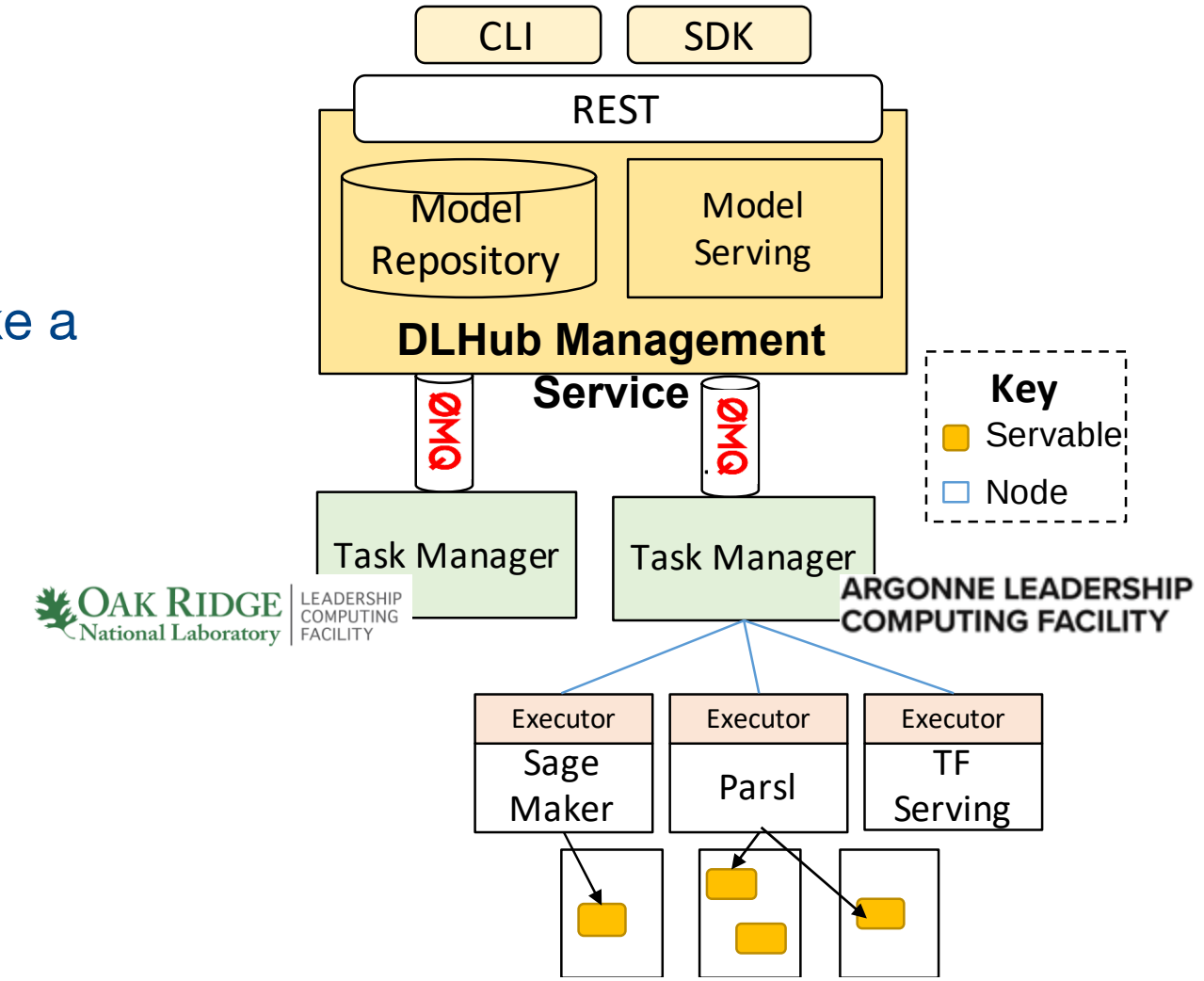
- REST API with Python SDK (available) / CLI (delivery in Nov. 2018)
  - Support model markup, data staging, registration, and invocation
- Model Repository
  - Container registry
  - Advanced search functions
  - Identifier minting capabilities



https://github.com/DLHub-Argonne

DLHub Architecture

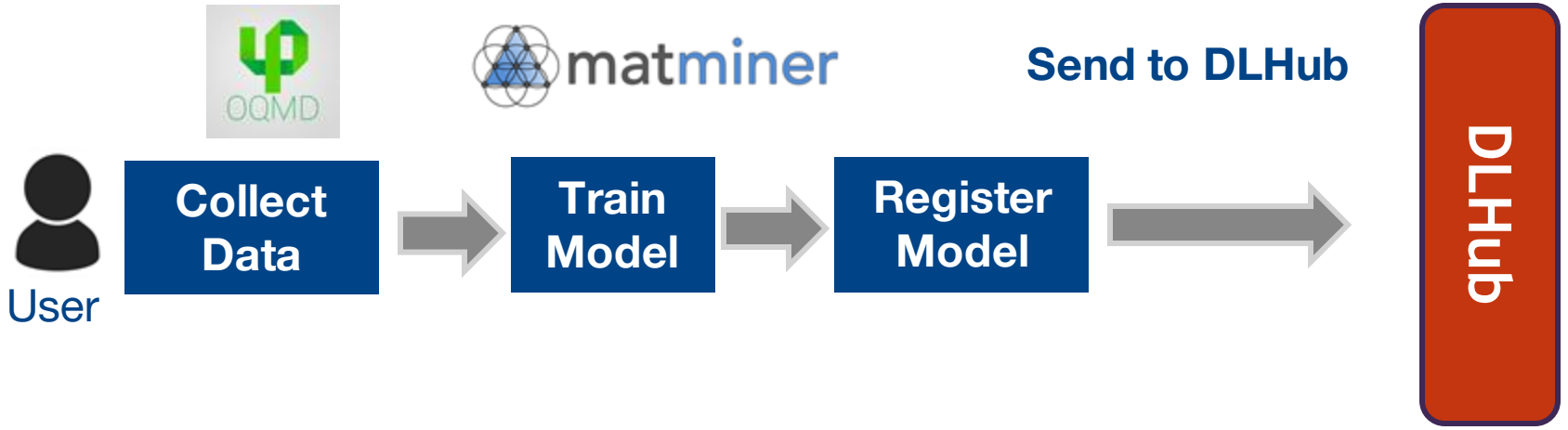
- Task Managers (TM) to support execution on various compute resources
- Executors chosen by TM to invoke a given servable'
- Caching at TM
- Data staging with Globus
- Batch submissions
- Scalability through deployment of model replicas



DLHub Model Registration and Publication

- **Register** model metadata, weights, and files to improve discoverability and reusability
- **Containerize** model to enhance interoperability
- **Identify** model with a permanent identifier (e.g., DOI, minid)
- **Version** model and data pre/post processing steps
- **Deploy** model with simplified interfaces for users
- **Control** access to model metadata and usage

- (future) **Automate** retraining and testing when new data are available



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Marking up a Model - Python SDK

Existing Model

User Mark Up with SDK

SDK Extracts Metadata for Known Model Types

Send to DLHub (via Globus or HTTPS)

DLHub Containerization

Populate Search Index / Mint Identifiers

```python
from dlhub_toolbox.models.servables.keras import KerasModel
import pickle as pkl
import json

# Describe the keras model
model = KerasModel('model.hd5', list(map(str, range(10))))

# Describe the model
model.set_title("MNIST Digit Classifier")
model.set_name("mnist_tiny_example")
model.set_domains(["general","digit recognition"])

# Add link to paper describing the dataset
model.add_related_identifier("10.1109/CVPR.2007.383157", "DOI",
                             "IsDescribedBy")

model.set_authors(["Lecunn, Yann", "Cortes, Corinna"])

# Describe the outputs in more detail
model.output['description'] = 'Probabilities of being 0-9'
model.input['description'] = 'Image of a digit'
```

Python SDK - Automated Metadata Generation

Citation Metadata

```
"datacite": {
    "creators": [{
            "givenName": "Yann",
            "familyName": "Lecunn",
            "affiliations": []
        },
        {
            "givenName": "Corinna",
            "familyName": "Cortes",
            "affiliations": []
        }
    ],
    "titles": [{
        "title": "MNIST Digit Classifier"
    }],
    "publisher": "DLHub",
    "publicationYear": "2018",
    "relatedIdentifiers": [{
        "relatedIdentifier": "10.1109/CVPR.2007.383157",
        "relatedIdentifierType": "DOI",
        "relationType": "IsDescribedBy"
    }],
    "identifier": {
        "identifier": "10.YET/UNASSIGNED",
        "identifierType": "DOI"
    },
    "resourceType": {
        "resourceTypeGeneral": "InteractiveResource"
    }
},
```

DLHub Metadata

```
"dlhub": {
    "version": "0.1",
    "domains": [
        "general",
        "digit recognition"
    ],
    "visible_to": [
        "public"
    ],
    "id": null,
    "name": "mnist_tiny_example",
    "files": {
        "other": [],
        "model": "model.hd5"
    }
},
```

Access Control

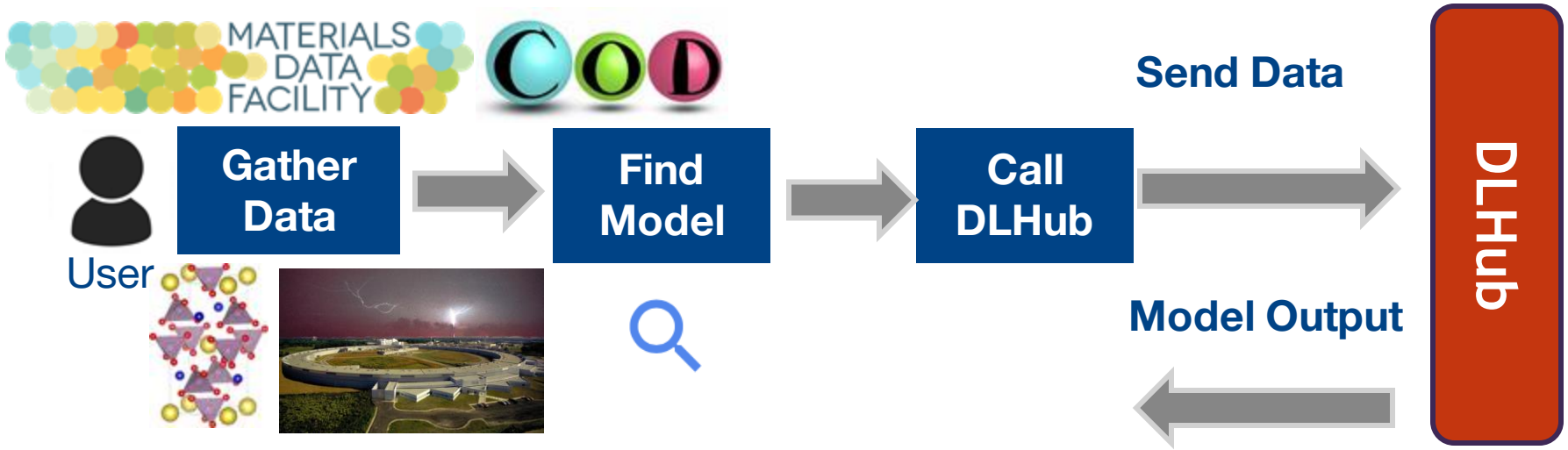
- Public
- Globus users
- Globus groups

Servable Metadata

```
"servable": {
    "methods": {
        "run": {
            "input": {
                "type": "ndarray",
                "description": "Image of a digit",
                "shape": [null,28,28,1]
            },
            "output": {
                "type": "ndarray",
                "description": "Probabilities of being 0-9",
                "shape": [null,10]
            },
            "parameters": {},
            "method_details": {
                "method_name": "predict",
                "classes": ["0","1","2","3","4",
                    "5","6","7","8","9"]
            }
        }
    },
    "shim": "keras.KerasServable",
    "language": "python",
    "dependencies": {
        "python": {
            "keras": "2.2.4",
            "h5py": "2.8.0"
        }
    },
    "type": "Keras Model",
    "model_type": "Deep NN"
```

DLHub Model Discovery and Usage

- Find curated and tested models
- Use models through simple interfaces



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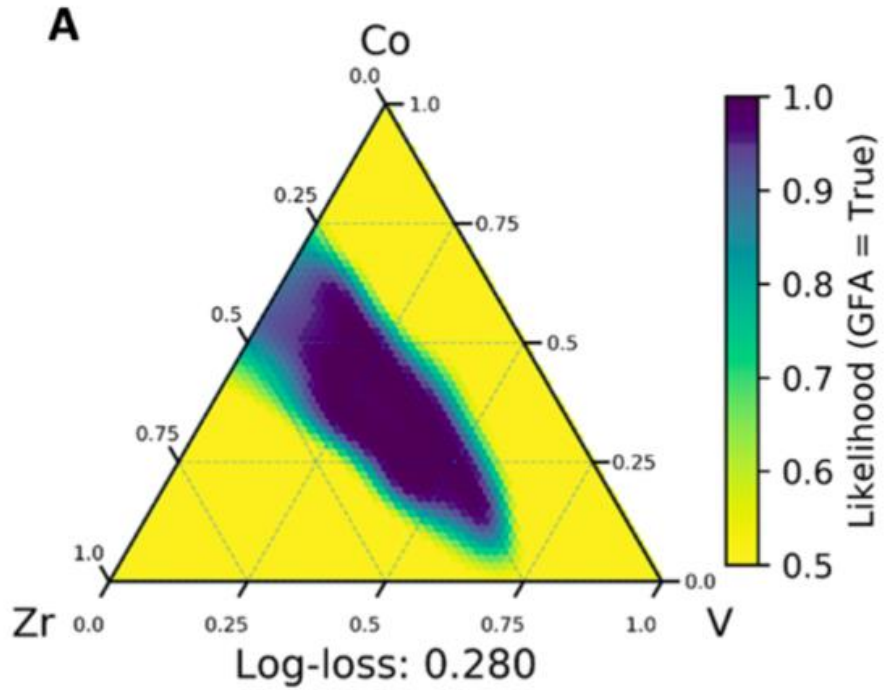
Predicting Glass-forming Ability

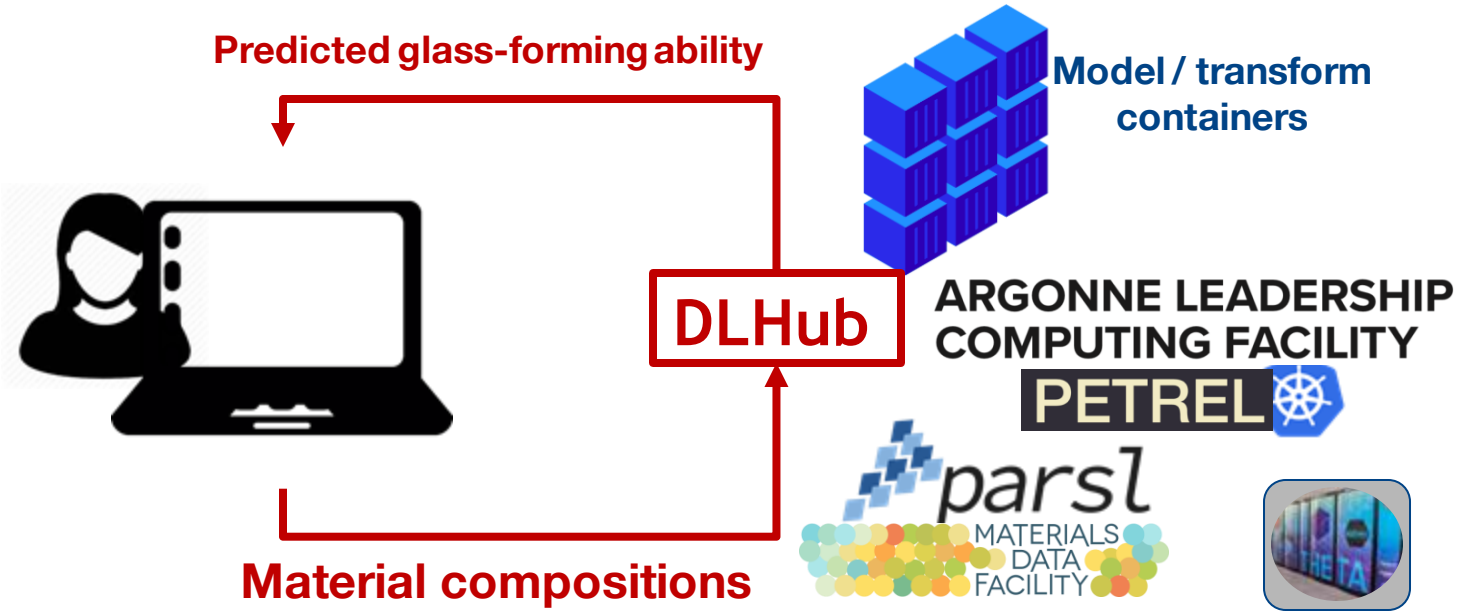
Accelerated discovery of metallic glasses through iteration of machine learning and high-throughput experiments

Fang Ren[1,*], Logan Ward[2,3,*], Travis Williams[4], Kevin J. Laws[5], Christopher Wolverton[2], Jason Hattrick-Simpers[6] and Apurva Mehta[1,†]

10.1126/sciadv.aaq1566



- Where are the model and trained weights?
- How do I run the model on my data?
- How can I retrain the model on new data?
- How can I build on this work?



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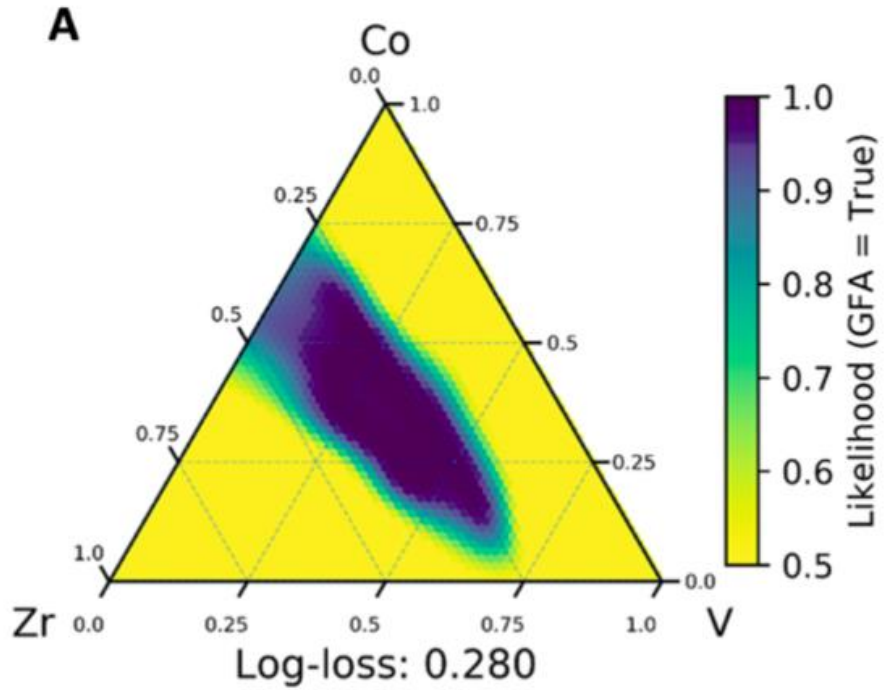
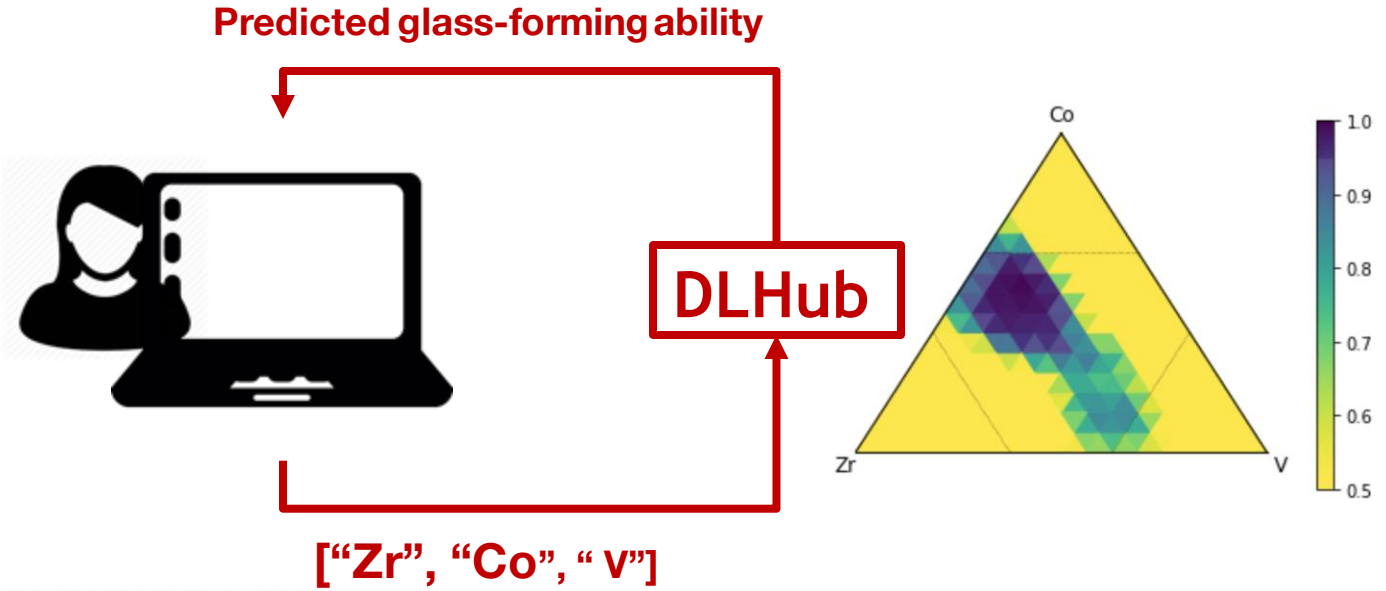



```
servable_name = "metallic_glass"
servable_id = dl.get_id_by_name(servable_name)
elems = ["V","Co","Zr"]

res = dl.run(servable_id, {"data":elems})
```



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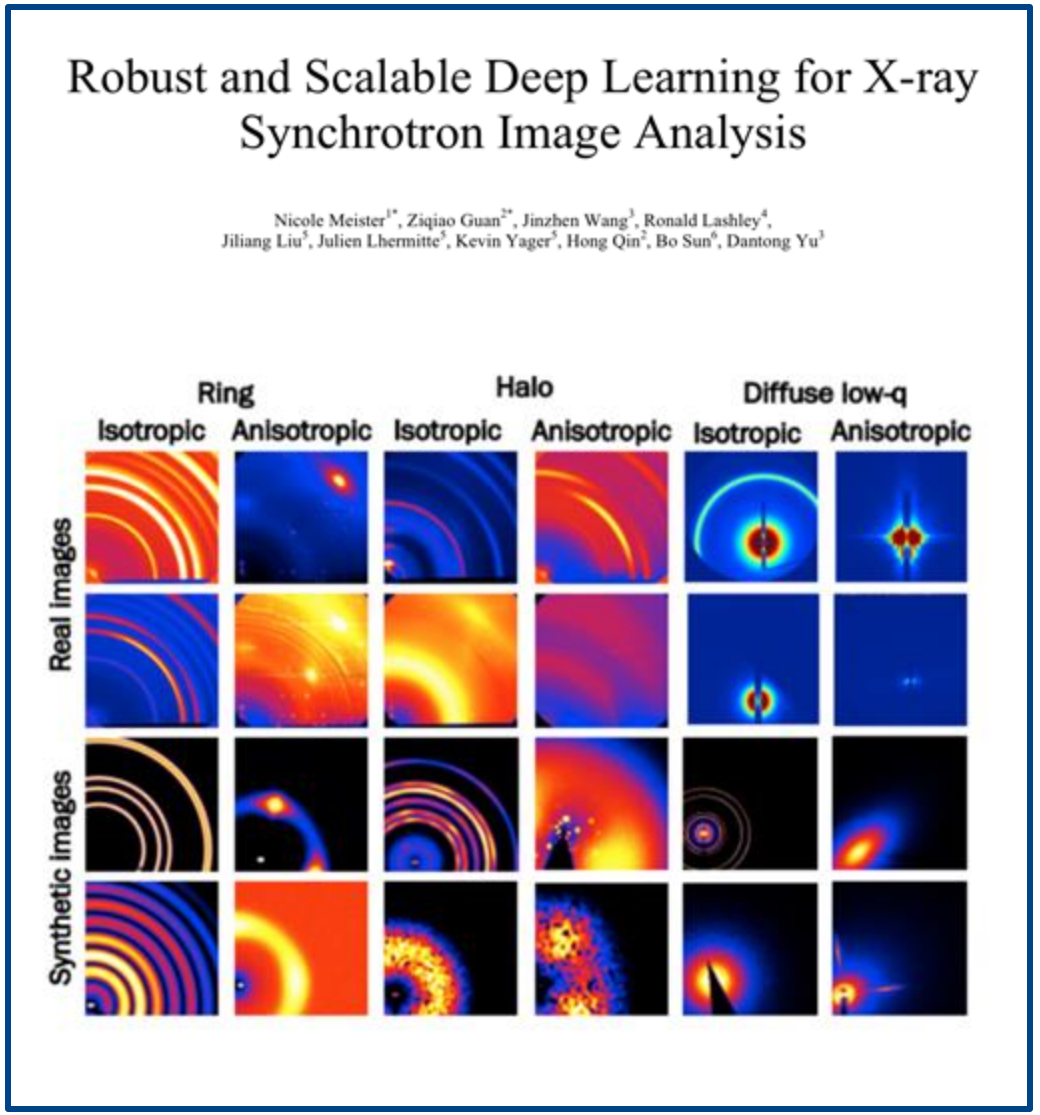
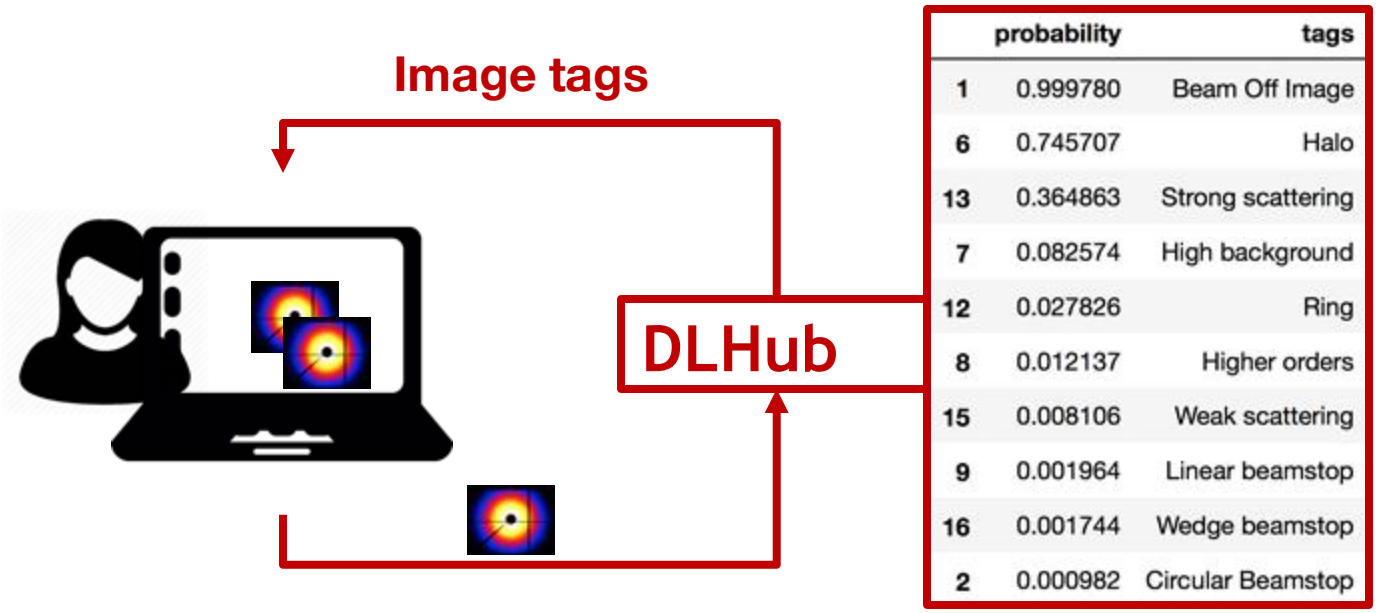
Analyzing Beamline Images



- Stage data into containers via Globus HTTPS
- Pass valid token and data location



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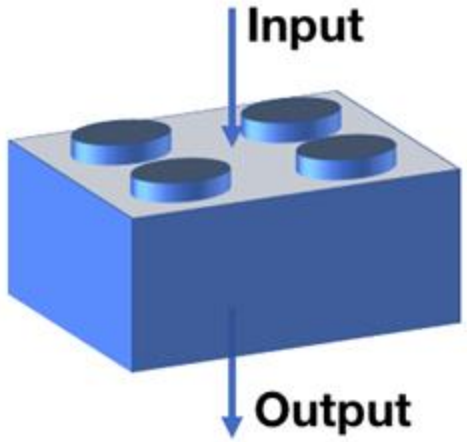
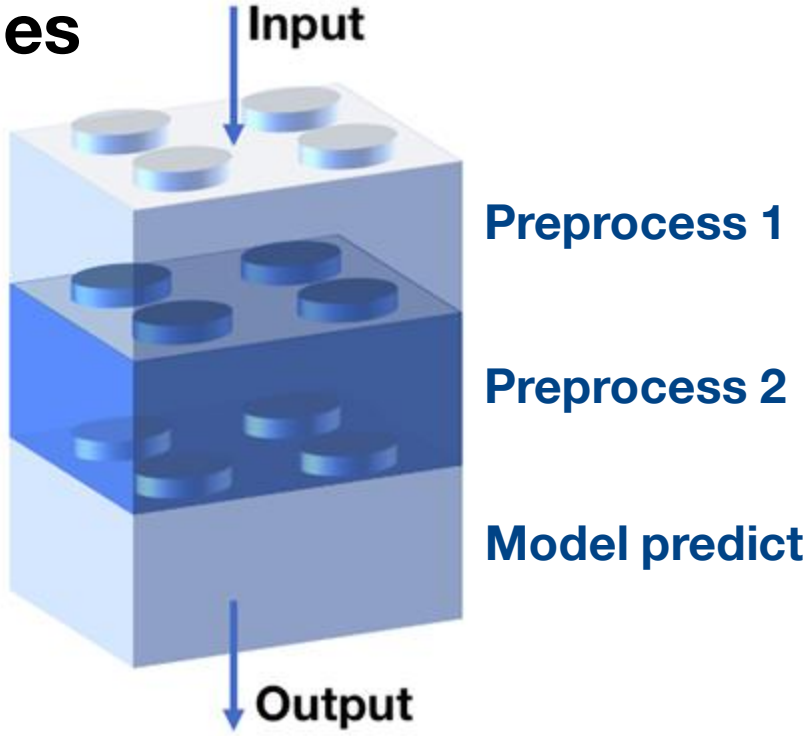
Data and Learning Hub (DLHub): Pipelines

Servables



Pipelines



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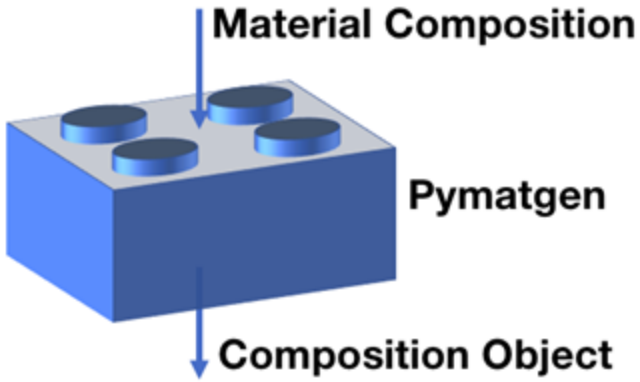
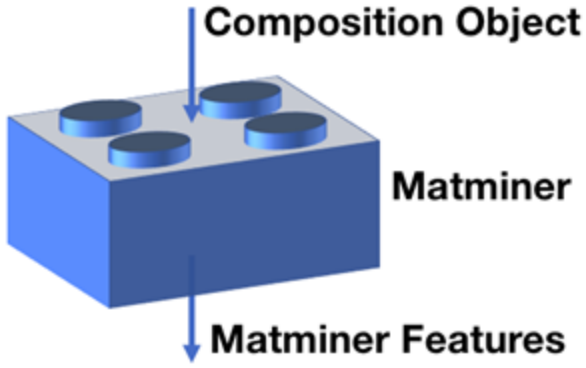
Pipelines: Predicting Formation Enthalpy

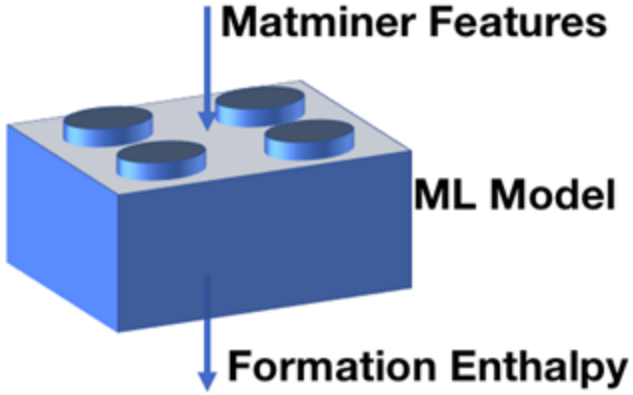
Step 1



Step 2



Step 3



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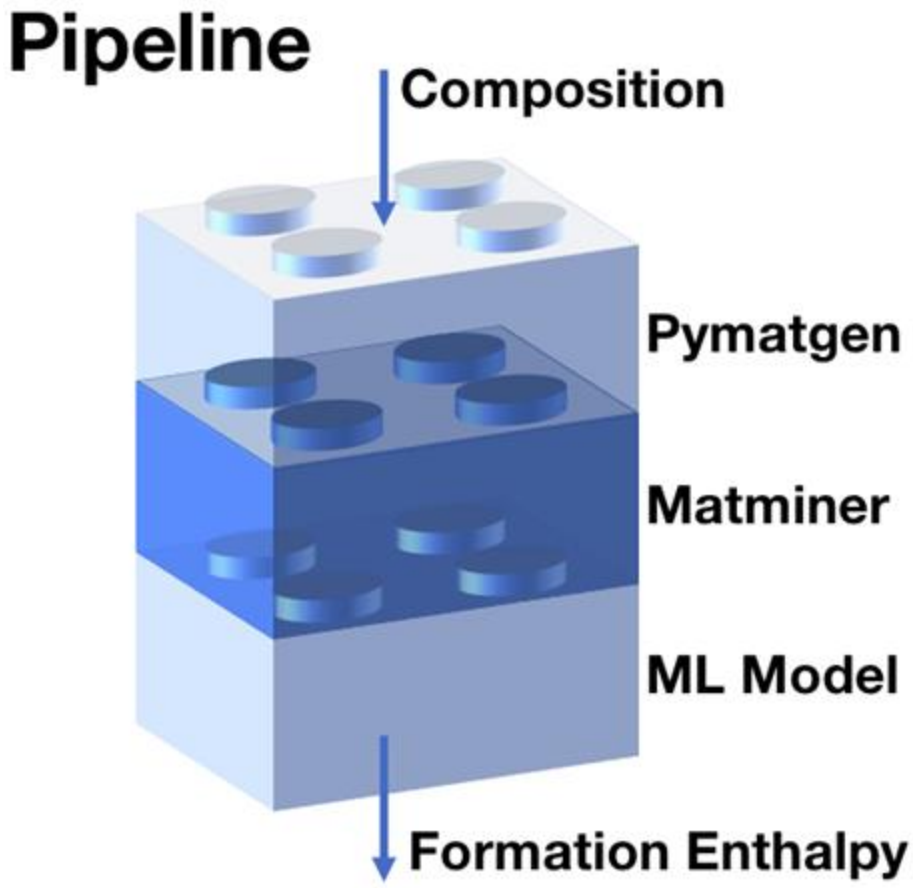
Predicting Formation Enthalpy



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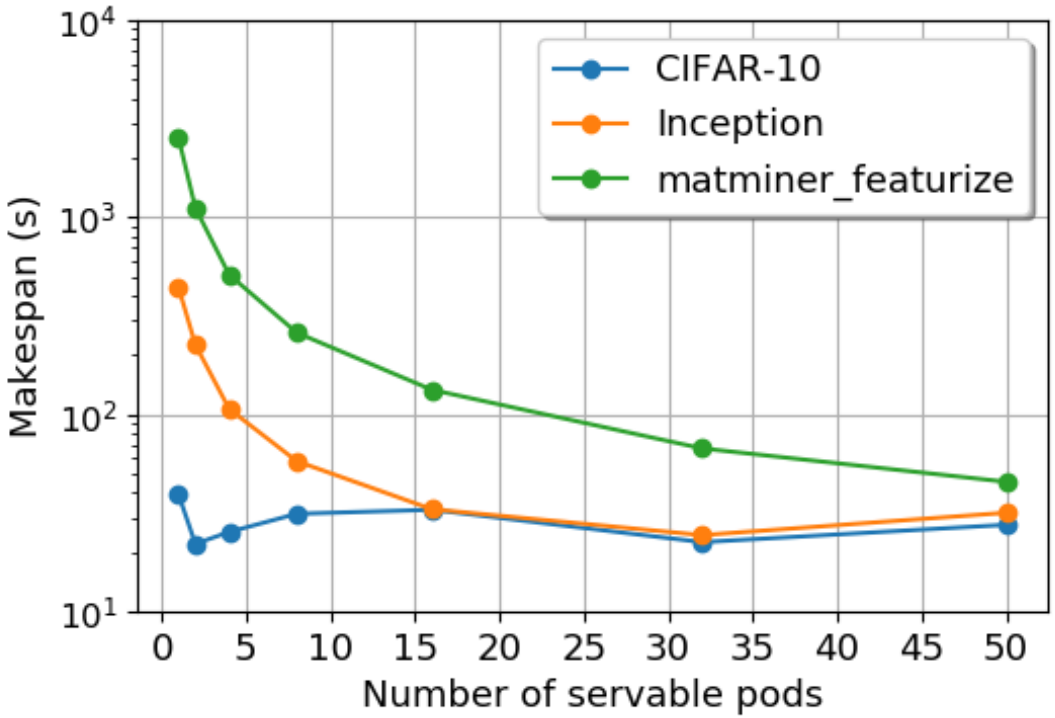
DLHub Performance

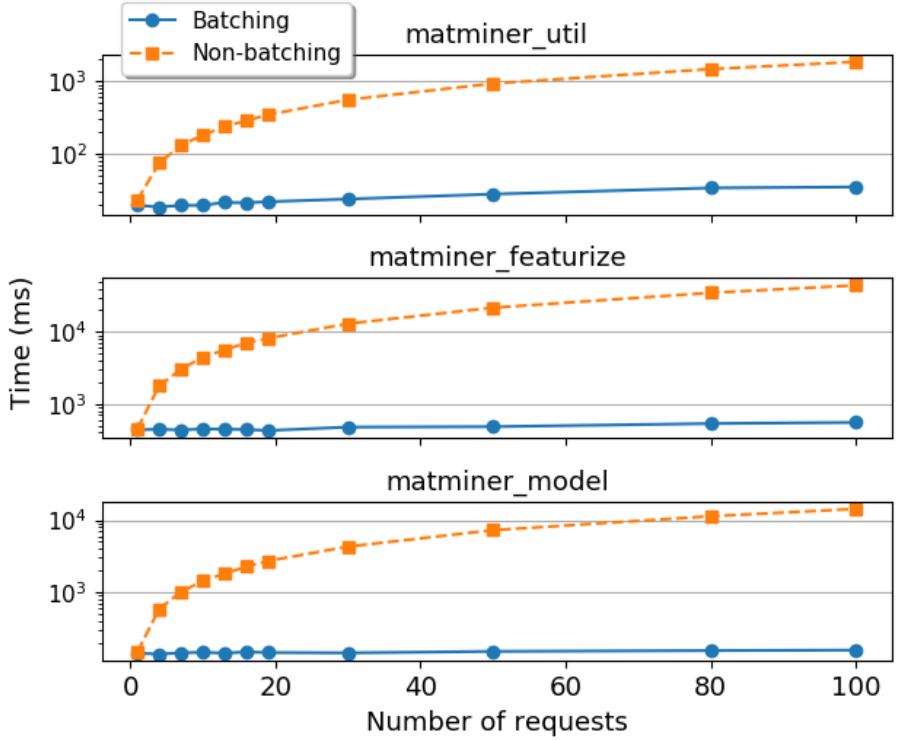
DLHub Performance

Scale Testing



The time required for the Inception, CIFAR10, and Matminer-featurize models to process 5000 inferences with varying numbers of replicas.

Batching



Servable invocation time, with and without batching.

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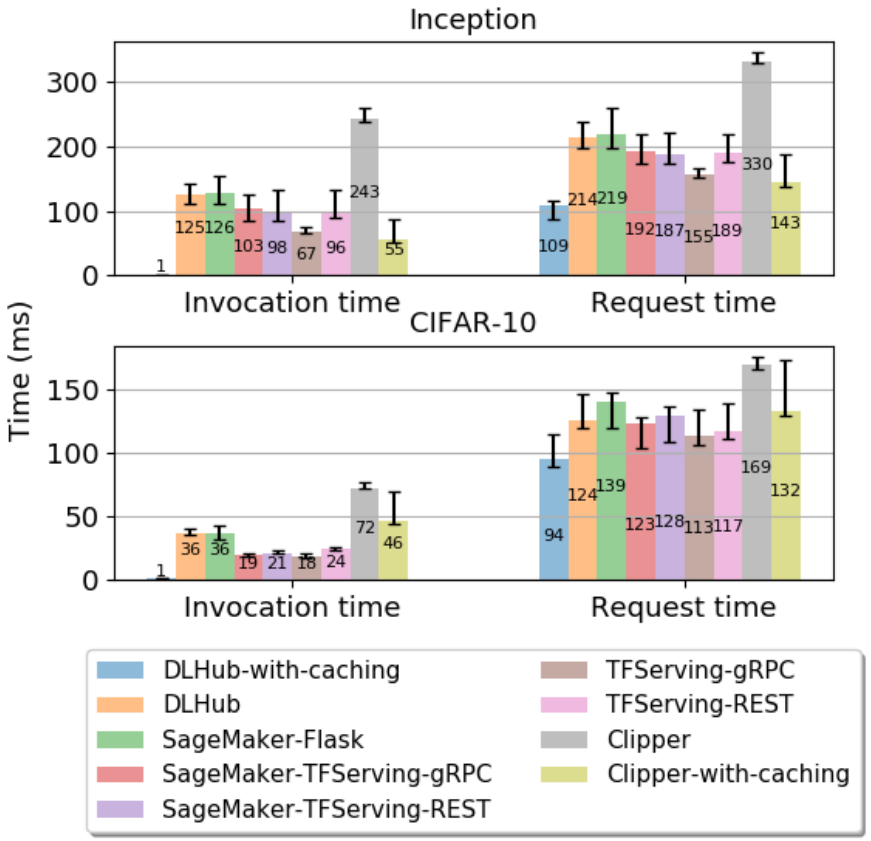
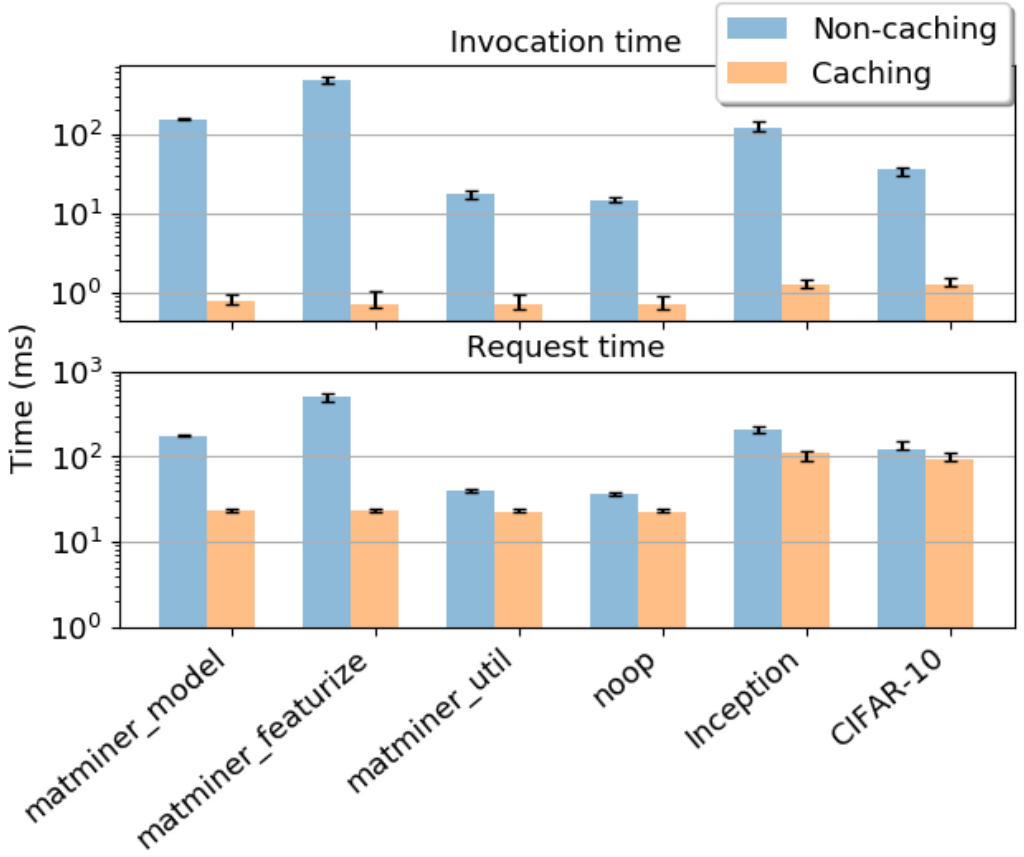
DLHub Performance

Serving General Models



Performance of different serving systems on the Inception and CIFAR-10 problems.

Caching



Performance impact of caching in DLHub. Bars and error bars show median and 5th/95th percentiles

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DLHub Summary

Model deposit and discovery

- Developed a model schema to promote discovery
- Implemented advanced search and filtering
- Built ingest flow: models are dynamically staged, packaged, dockerized, published, and indexed

Model serving

- Deployed capabilities for users to run inference with SDK and CLI
- Automated testing of containers
- Implemented caching and batching

Support for multiple execution sites

- PetrelKube: Parsl, TF serving, Sagemaker
- Other: AWS, OSG

Authentication

- Protected model metadta and inference with GlobusAuth
- Secured data staging

Monitoring and statistics

- Request, invocation, data staging

Future work

- Dynamic scaling by load
- Build Web UI to create pipelines and invoke models
- Cache at the servable level within pipelines
- Couple DLHub to data sources (MDF, etc.)
- Integrate with ML frontend tools (DeepForge), optimization tools (DeepHyper), and more
- Create interface for training and retraining of models

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Data Management and Sharing Pilot

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MATERIALS DATA FACILITY

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DLHub

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