Transformative Applications of Materials Data Science:

Spatiotemporal Studies, Graph & Deep Learning To Solve Materials Challenges

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A selection of Lifetime Extension Articles

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http://dmseg5.case.edu/people/faculty.php?id=rxf131

A BHEF CASE STUDY

CREATING A MINOR IN

APPLIED DATA SCIENCE

Case Western Reserve University Engages Business Leaders to Produce T-Shaped Professionals

THROUGH THE COLLABORATION of its business and higher education members, the Business-Higher Education Forum (BHEF) launched the National Higher Education and Workforce Initiative (HEWI) to create new undergraduate pathways in high-skill, high-demand fields such as data science and analytics. Data science and analytics must be integrated with T-shaped skills, such as critical thinking, collaboration, and effective communication, which are critical for all graduates entering the 21st century workforce. Knowledge of data science and analytics in recent years has become as fundamental as any other skill for graduates' career readiness. BHEF's Strategic Business Engagement Model with higher education addresses this demand by moving the two sectors from transactional relationships to strategic partnerships through five strategies:

1. **ENGAGE** corporate leadership;
2. **FOCUS** corporate philanthropy on undergraduate education;
3. **IDENTIFY** and tap core competencies and expertise;

undergraduate education.

This case study examines how BHEF member Case Western Reserve University (Case Western Reserve) is integrating T-shaped skills into a minor in applied data science.

PROGRAM OVERVIEW

THE APPLIED DATA SCIENCE (ADS) MINOR AT CASE WESTERN RESERVE serves as a national model for undergraduate education in data science. Available to every undergraduate student across all schools at the university, this program of study requires experiential learning opportunities, embeds T-shaped skills, and allows students to master fundamental ADS concepts in their chosen domain area. From strong leadership engagement to funded undergraduate research opportunities, Case Western Reserve applied BHEF's Strategic Business Engagement Model to create a minor that responds to the fundamental need for data science in today's global business community.

AY 2014-15	AY 2015-16	AY 2016-17	AY 2017-18	AY 2018-19	AY 2019-20	AY 2020-21	AY 2021-22	AY 2022-23	Total
9	36	49	57	100	106	92	159	102	710

Medical Mutual of Ohio
Medtronic
Philips Healthcare
Sherwin-Williams Company
Siemens
Teradata Corporation
Timken Company
University Hospitals

2

http://www.bhef.com/publications/creating-minor-applied-data-science

BHEF BUSINESS HIGHER EDUCATION FORUM
Creating Solutions. Inspiring Action.

lle.case.edu

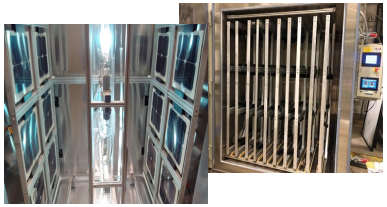
Service Lifetime Prediction (SLP): a PV example

Accurate PV SLP, is crucial to LCOE, and is the basis of PV lifetime performance

- Challenge: **PV modules are complex systems** with **multiple degradation mechanisms**

Requires:comprehensive study protocol development and data on variants and exposures

Our solution: mapping of degradation mechanisms and pathways with network modeling



Service Life Prediction:
In Lab ⬆️ & Field ⬇️

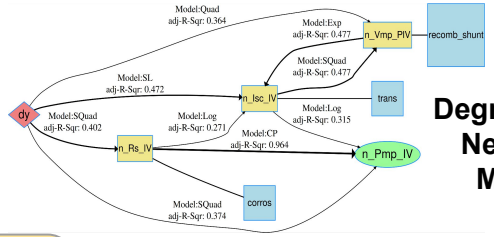
PV module variants :
BOM
Quality
Design

Weathering exposure stressors:
Climate
Racking

Cell technology
Encapsulation
Glass/Backsheet
Brand/Suppliers
Irradiance/UV
Moisture
Temperature

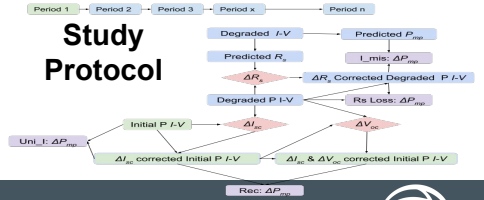
Degradation Network models

ΔR_s, corrosion
ΔI_{sc}, optical
ΔV_{mp}, *recombination*



Degradation Network Model

Study Protocol



Common Research Analytics & Data Lifecycle Environment

CRADLE Analytics & Compute Cluster

Distributed & High Performance Computing[1]

FAIRification of Datasets

1. A. Khalilnejad, et al., Automated Pipeline Framework for Processing of Large-Scale Building Energy Time Series Data, PLOS ONE. 15 (2020) e0240461. https://doi.org/10.1371/journal.pone.0240461.

Data Processing Framework: CRADLE

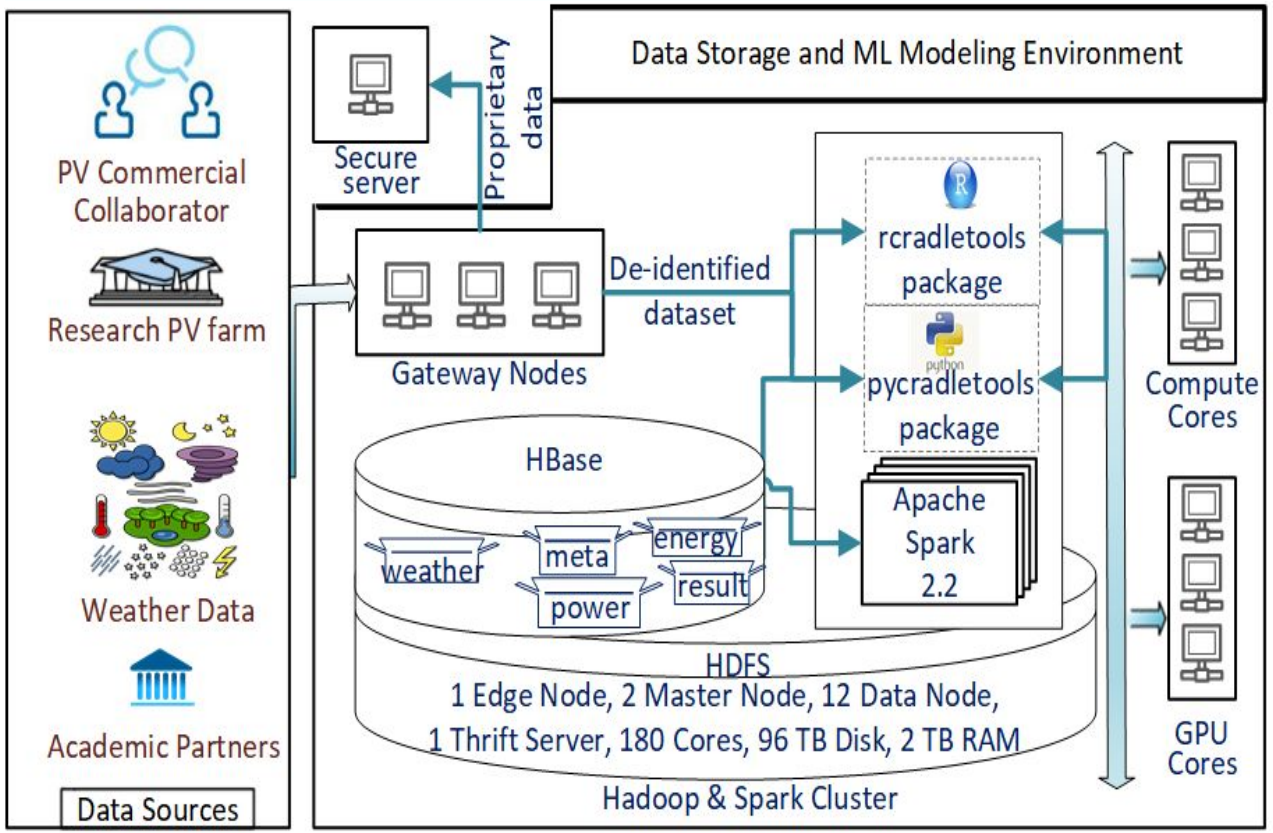
Data acquisition
- Diverse sources
- Anonymization
- Pre-processing
- Metadata

NoSQL Database system
- HBase

Computation
- Data Ingestion & Analysis
- Impute missing values
- R & Python3
- Tensorflow2
- Torch & Pytorch

CRADLE tools
- R & Python package
- Containerized Applications

Common Research Analytics & Data Processing Environment



CRADLE Compute Environment

Running in CWRU HPC
- **Rider (RHEL7)**
- **Pioneer (RHEL8 OS)**
- **Markov (Teaching Cluster)**

OnDemand Containerized Apps
- Using Ubuntu 20.04 OS

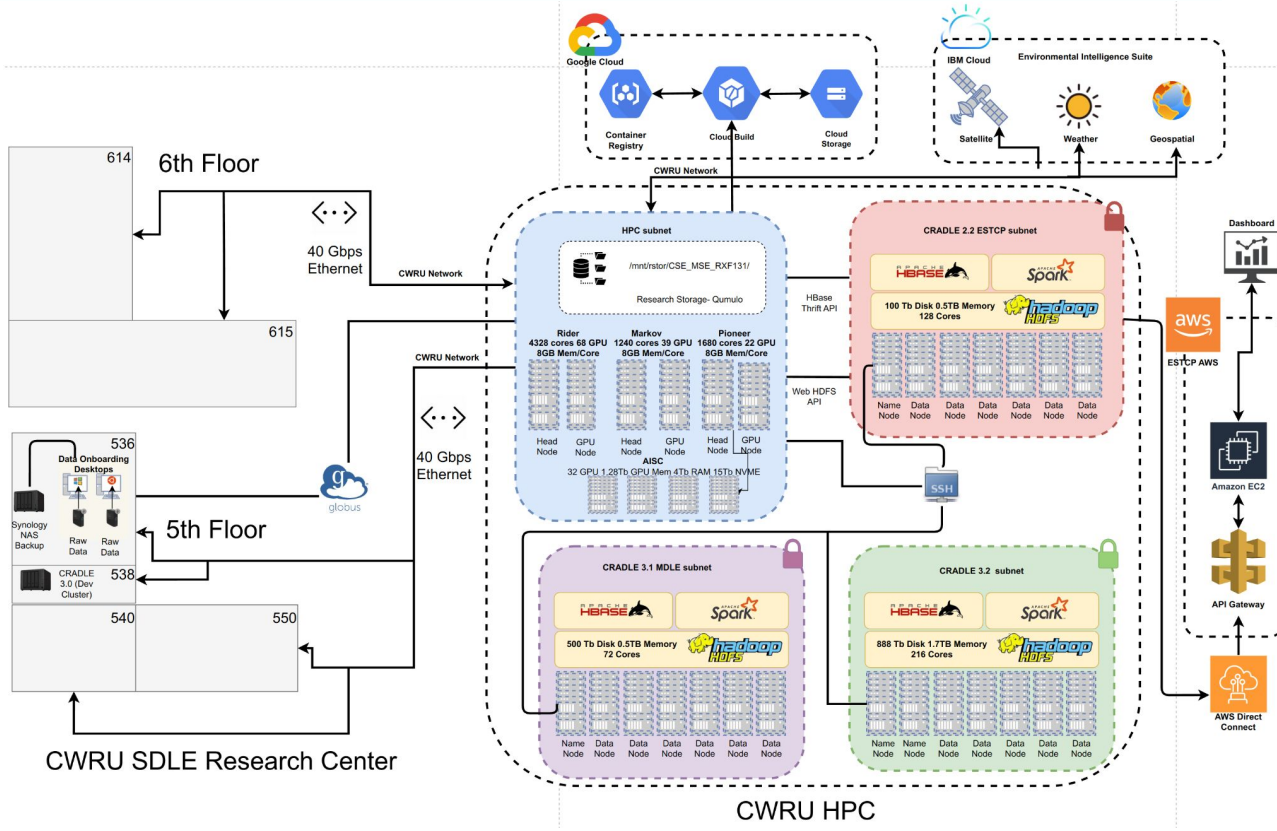
Cloudera Data Platform
- Comm. supported distribution
- Of Apache Hadoop/Hbase/Spark/….

2 Petabytes of Distrib. Comp. Storage
- **Meeting NIST 800-171 level 1**
- **For Controlled Unclassified Data**

Nvidia AISC
- 32 A100 GPU (40 Gb vRAM each)
  - = 1.28 Tb of GPU vRAM
- With 15 Tb of NVME Fast Storage

Able to train 100s of Deep Learning Models

Common Research Analytics & Data Processing Environment



CRADLE Analytics Environment

CRADLE 2.3
- 128 Cores
- 0.5 Tb RAM
- 100 Tb Storage
- CDH 5.16.2, SP-800-17

CRADLE 3.1
- 72 Cores
- 576 Gb RAM
- **480 Tb Storage**
- CDP 7.1, SP-800-171

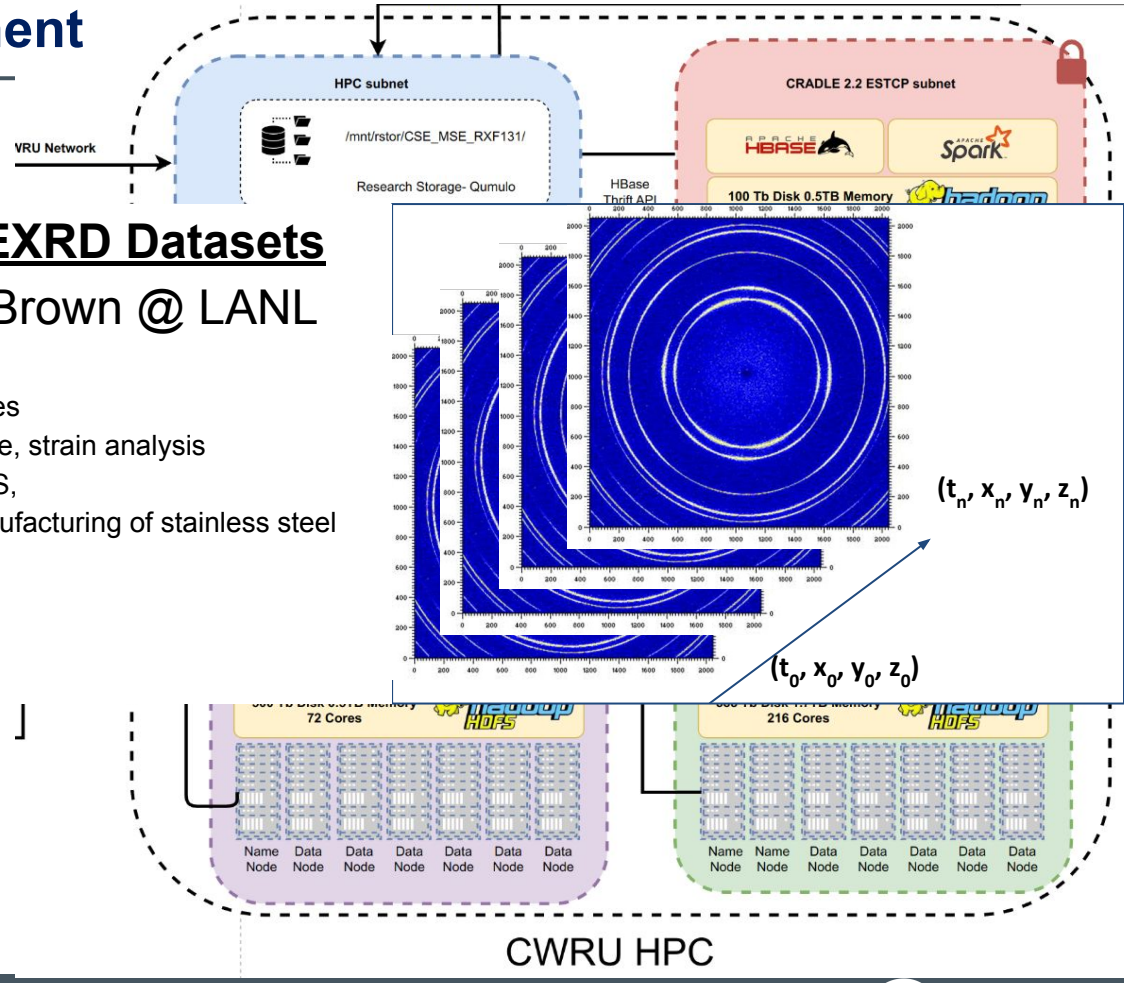
CRADLE 3.2
- 216 Cores
- 1.8 Tb RAM
- **1.5 Pb Storage**
- CDP 7.1, SP-800-171

NVIDIA GPU AISC
- 32 DGX A100 GPUs
  - 40 Gb RAM each
- **1.28 TB GPU RAM**
- **15 Tb NVME storage**

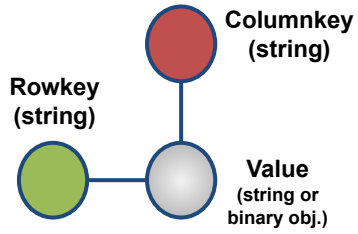
Current 2D-HEXRD Datasets

from Don Brown @ LANL

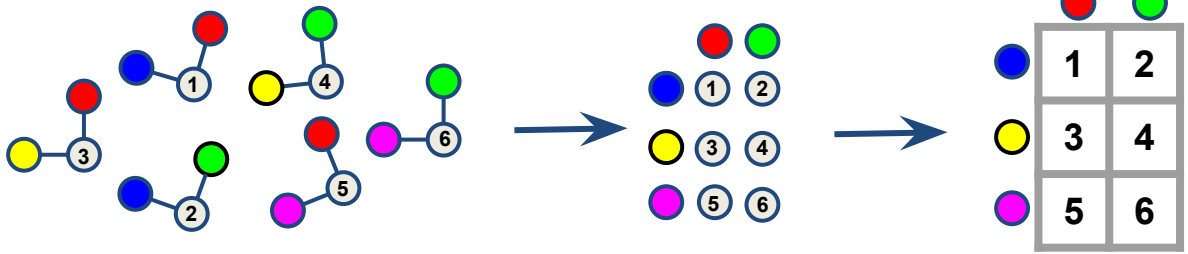
- ~ 13 Tb
- ~ 3 million XRD images
- In-situ heating, texture, strain analysis of Ti-6Al-4V at CHESS,
- Wire arc additive manufacturing of stainless steel etc.



The “NoSQL” Database Abstraction of Hadoop/Hbase: RDF Triples



HBase RDF ‘Triple’



Combines Lab data (Spectra, Images, Videos etc.)

With Geospatiotemporal Data (PV Power Plant Data)

Distributed & High Performance Computing:

Petabyte Data Lake In A Petaflop HPC Environment

- In-place Analytics: Distributed Spark Analytics in Hadoop/HDFS/Hbase
- In-memory Data Extraction: To Separate HPC Compute Nodes

A non-relational data warehouse for the analysis of field and laboratory data from multiple heterogeneous photovoltaic test sites

Yang Hu, *Member, IEEE,* Venkat Yashwanth Gunapati, Pei Zhao, Devin Gordon, Nicholas R. Wheeler, Mohammad A. Hossain, *Member, IEEE,* Timothy J. Peshek, *Member, IEEE,* Laura S. Bruckman, Guo-Qiang Zhang, *Member, IEEE,* and Roger H. French, *Member, IEEE*

Automated pipeline framework for processing of large-scale building energy time series data

Arash Khalilnejad[1,5], Ahmad M. Karimi[2,5], Shreyas Kamath[1,5], Rojiar Haddadian[2,5], Roger H. French[2,4,5]*, Alexis R. Abramson[3,6¤]

Compute and data

HPC Cluster

Rider

- 4328 cores
- 68 GPU
- 8 Gb Mem/core

Markov

- 1240 cores
- 39 GPU
- 8 Gb Mem/core

Pioneer

- 1680 cores
- 22 GPU
- 8 Gb Mem/core

Hadoop Cluster

CRADLE 2.1

- 75 TB
- 192 cores
- 1TB memory
- 15 nodes

CRADLE 2.2

- 100 TB
- 128 cores
- 500GB memory
- 4 nodes

CRADLE 3.1

- 500 TB
- 72 cores
- 564GB memory
- 3 nodes

Data

Temporal data:

- ~2000 PV power plant data
- ~1000 Buildings energy consumption
- ~1000 Locations with weather data

Geospatial data:

- ~1200 Well data
- ~1000 Locations with subsurface temperature

XCT data: 50 TB

- Diamond Light Source
- LLNL

XRD data: ~12TB

Singularity containers

Portable and reproducible containers

- **Cybersecure**
- **Admin privileges not required**
  - Different from Docker Containers

Easy to resolve software dependency conflict

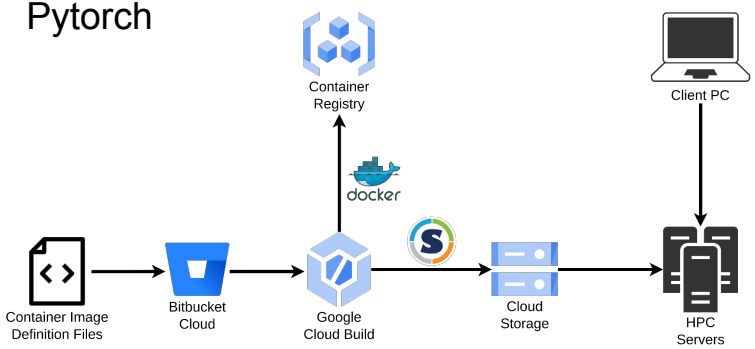
- NVIDIA CUDA
- Python version

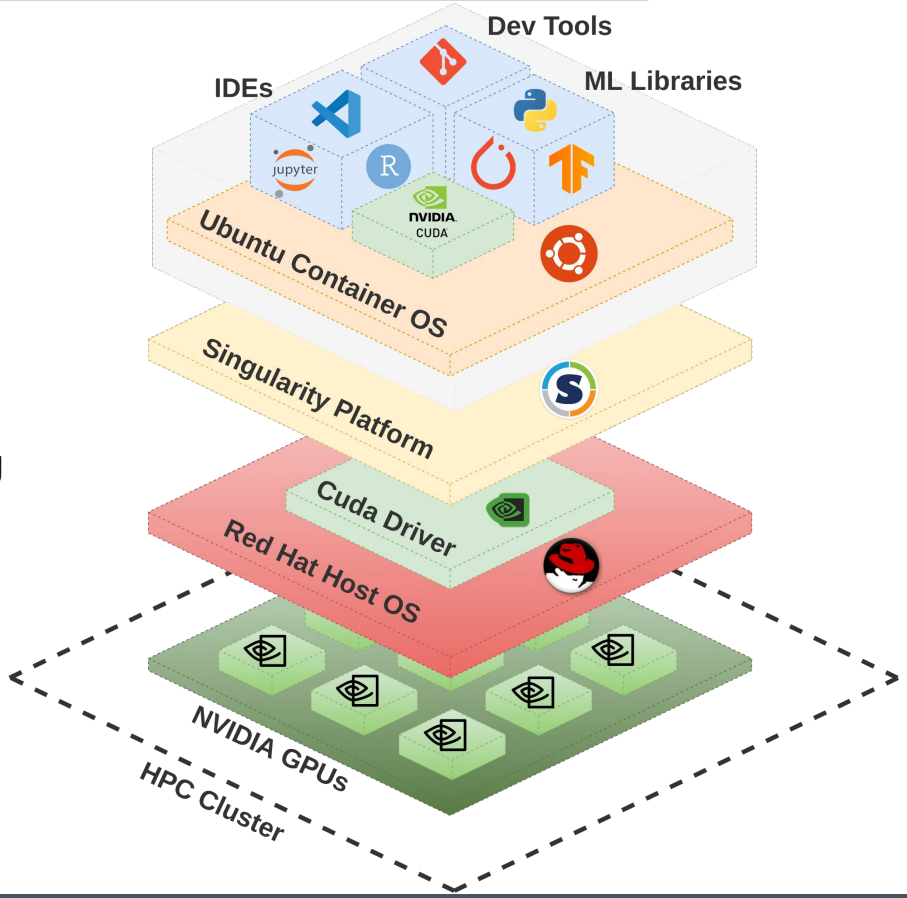
Ubuntu 20.04lts Based container

- Supports all major data science packages

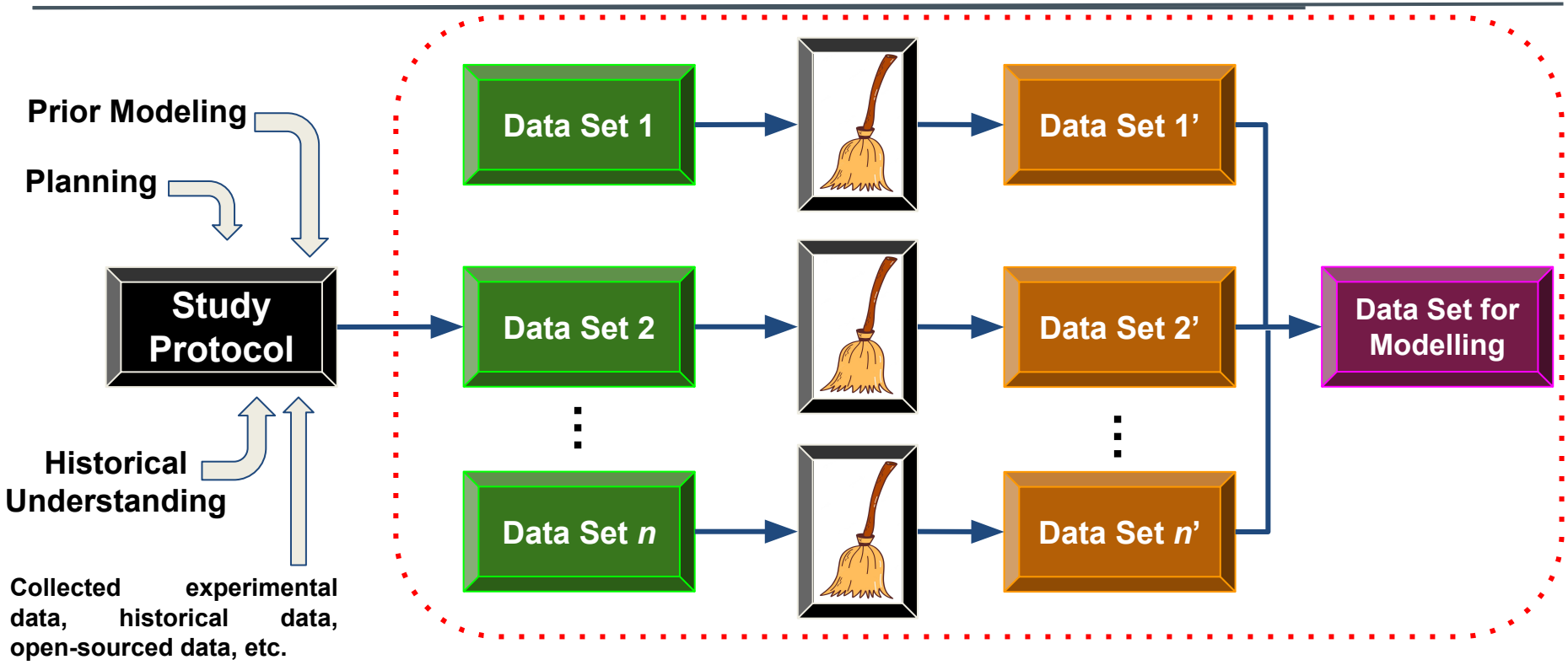
Enables multi-GPI Deep neural network training

- Tensorflow
- Pytorch



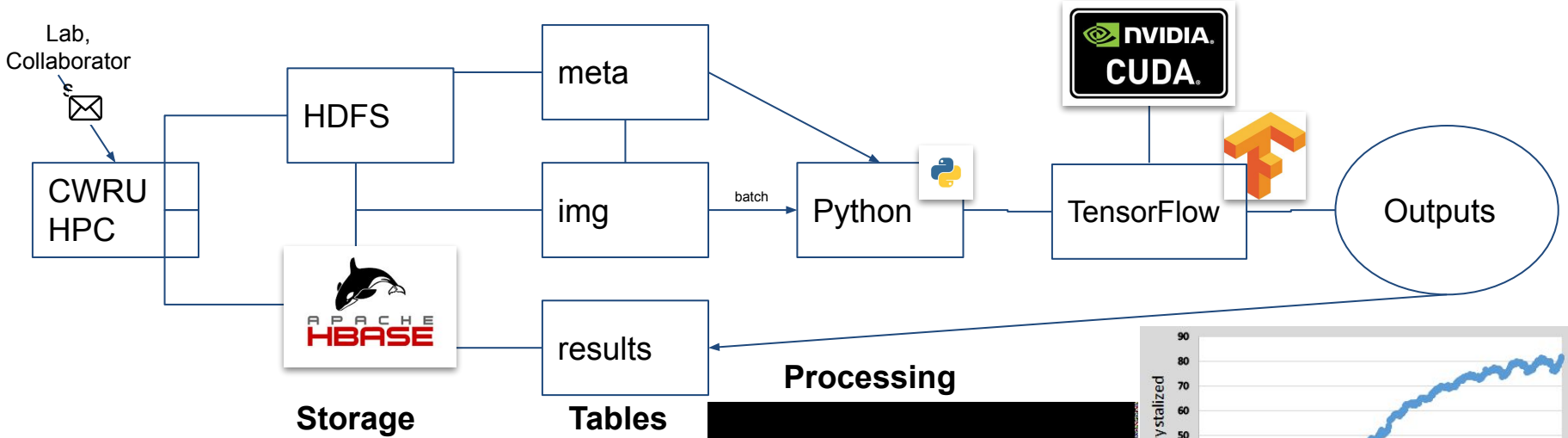


Data Science Pipelining



Poor data and experimental planning can have embarrassing/catastrophic outcomes: [1], [2]

Data Processing Infrastructure: A Data Analysis Pipeline (Python or R)



CRADLE infrastructure

NoSQL database

- Apache HBase

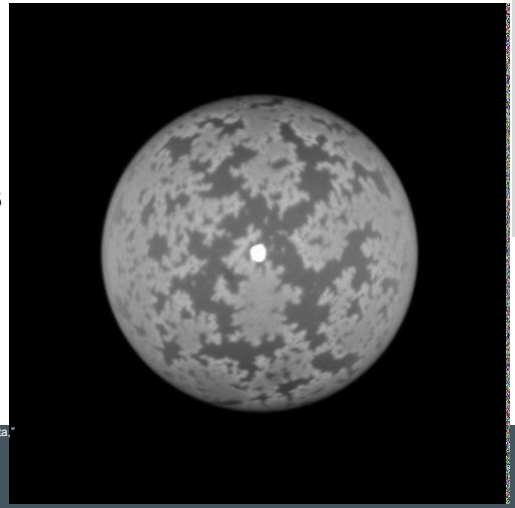
HPC environment

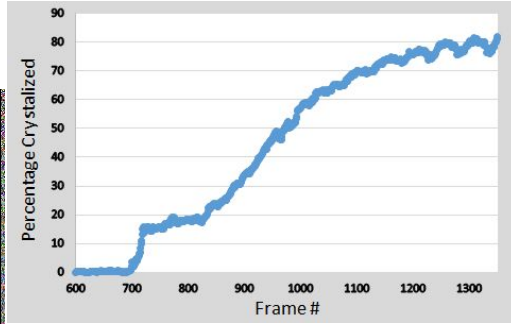
- Nvidia GPU acceleration for deep learning

Python/TensorFlow language

Nucleation & Growth of AlN Crystals

- From Al/Ni Melt
- 1 Million Images





M. Adachi, S. Hamaya, D. Morikawa, B. G. Pierce, A. M. Karimi, Y. Yamagata, K. Tsuda, R. H. French, H Fukuyama, Temperature dependence of crystal growth behavior of AlN on Ni–Al using electromagnetic levitation and computer vision technique", Mat. Sci. in Semicon. Proc., 153, 2023, 107167, ISSN 1369-8001, https://doi.org/10.1016/j.mssp.2022.107167
.

[1] A. Khalilnejad, et al., "Automated Pipeline Framework for Processing of Large-Scale Building Energy Time Series Data," PLOS ONE, p. e0240461, Dec. 2020, https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0240461 .
[2] Masayoshi Adachi et al., "In-situ observation of AlN formation from Ni-Al solution using an electromagnetic levitation technique," J Am Ceram Soc, p. jace.16960, Jan. 2020, https://onlinelibrary.wiley.com/doi/abs/10.1111/jace.16960 .

FAIRification of Datasets & Models, Enables AI learning

Making Datasets & Models FAIR

- By “FAIRification”

Enables Models to find Data

- And Data to find Models

So that they can advance

- Without human intervention

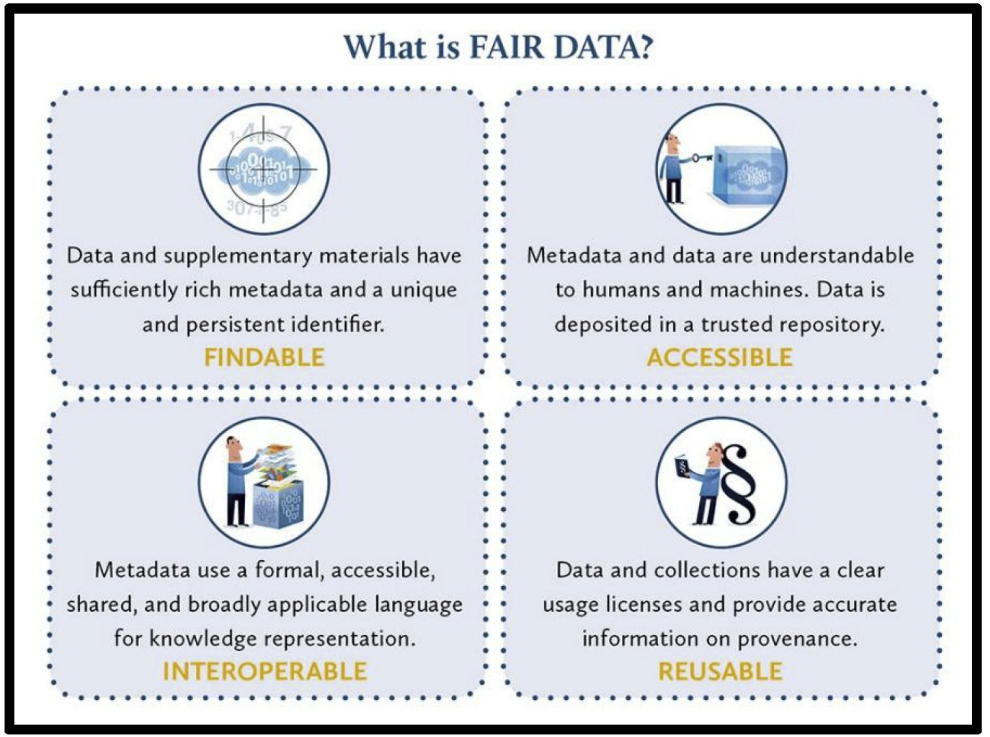
This is an aspect of the Semantic Web

- And Resource Description Framework
- Hbase triples are an example of RDF

FAIRification essential to
DOE SETO AI awards

- For st-GNN, that includes FAIRification
- And PV Multiscale

DOE-NNSA: Materials Degr. & Life Ext.
IEA-PVPS Task 13



M. D. Wilkinson et al., “The FAIR Guiding Principles for scientific data management and stewardship,” Sci. Data, vol. 3, no. 1, pp. 1–9, Mar. 2016, doi: 10.1038/sdata.2016.18.
https://en.wikipedia.org/wiki/Resource_Description_Framework

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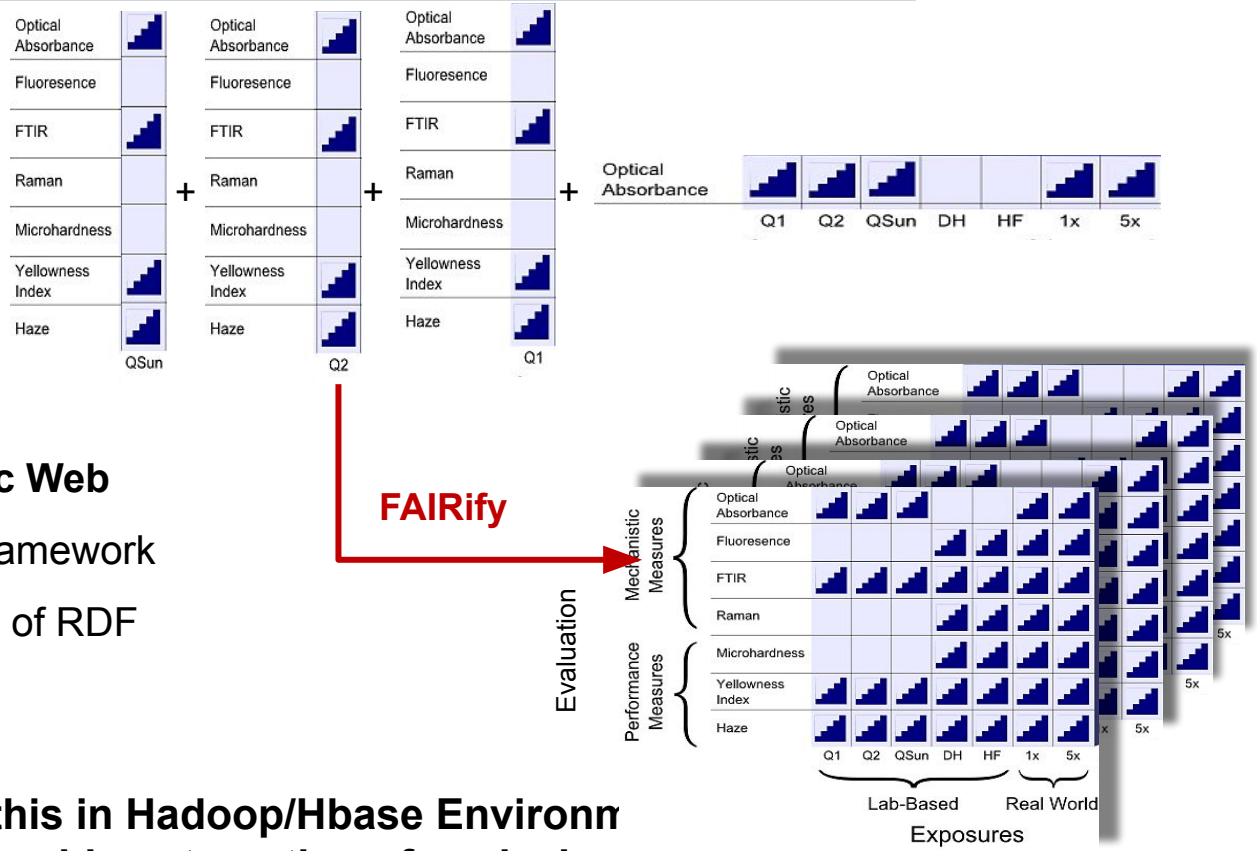


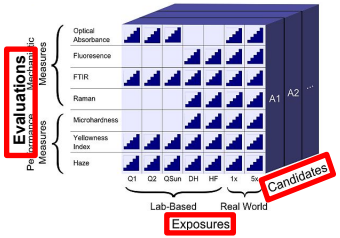
Enabling this in Hadoop/Hbase Environm

- **Can enable automation of analysis**

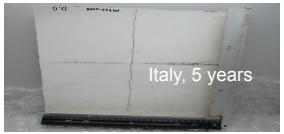
M. D. Wilkinson et al., “The FAIR Guiding Principles for scientific data management and stewardship,” Sci. Data, vol. 3, no. 1, pp. 1–9, Mar. 2016, doi: 10.1038/sdata.2016.18.
https://en.wikipedia.org/wiki/Resource_Description_Framework

Lifetime & Degradation Science Framework and Thrusts

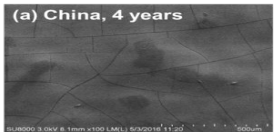
Exposures & Evaluations of Fielded Materials & Components

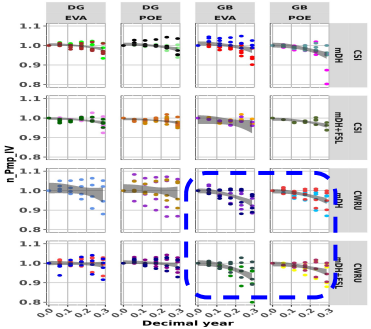


Forensic Studies on Field-Retrieved Components



PV Module Cracked Backsheets





Lifetime Performance of eight PV Mini-module Variants

Lab-based Accelerated Studies

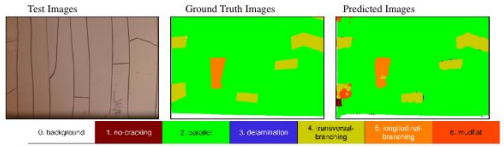
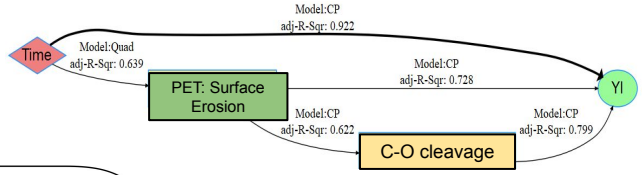
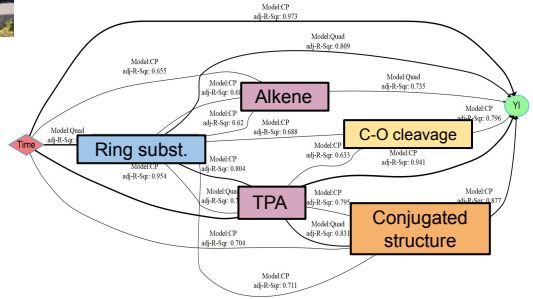


Figure 8. Six examples of crack inspection task performed on the test images using the trained Model O. The different colors in the (b) and (c) column images indicated different crack classes shown in the color bar.

CNN Classification of Accelerated Exposed Backsheet Cracks

Network models: <*S*|*M*|*R*> Mechanistic Degradation Pathway





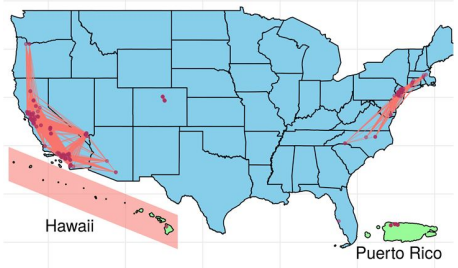
PET Degradation

Under accelerated exposures with water spray (top) and humidity (bottom)

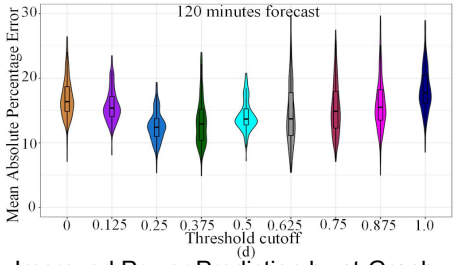
Chemical degradation mechanisms Identified along pathways

Surface erosion with spray.

Deep Learning with spatiotemporal-Graph Modeling



st-Graph Neural Network Models



Improved Power Prediction by st-Graph Neural Network Model

Lyu, Y., et. al. *Solar Energy*, 199, 425-436. Zhang, B., et al. (2019). *Scientific reports*, 9(1), 1-13. J. Liu *et al.*, *2020 47th IEEE Photovoltaic Specialists Conference (PVSC)*, Calgary, OR, 2020, pp. 1709-1714. A. Karimi, et al., *Proc. IAAI-21*, 2021. Yang, H. E., French, R., & Bruckman, L. (Eds.). (2019). *Durability and Reliability of Polymers and Other Materials in Photovoltaic Modules*. William Andrew.

Knowledge Graphs

Spatiotemporal Graphs

And Their Role in

Deep Representation Learning

Knowledge graphs: Nodes & Edges Define Relationships

What is a knowledge Graph?

- **Nodes:** entities w. types & attributes;
- **Edges:** relations
- capture (factual) knowledge as graphs

Where do KGs come from?

- Structured data: sensors, tables, Wiki infoboxes,
  databases, social nets, …
- Unstructured data: text, images, videos

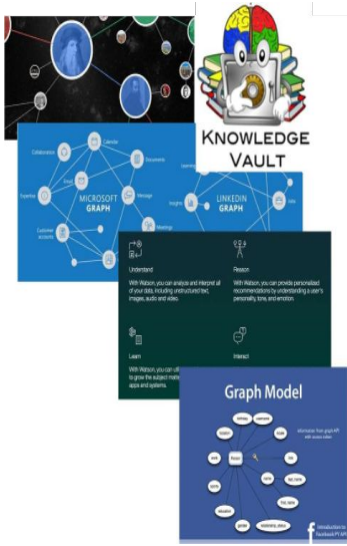
Why (Knowledge) Graphs?

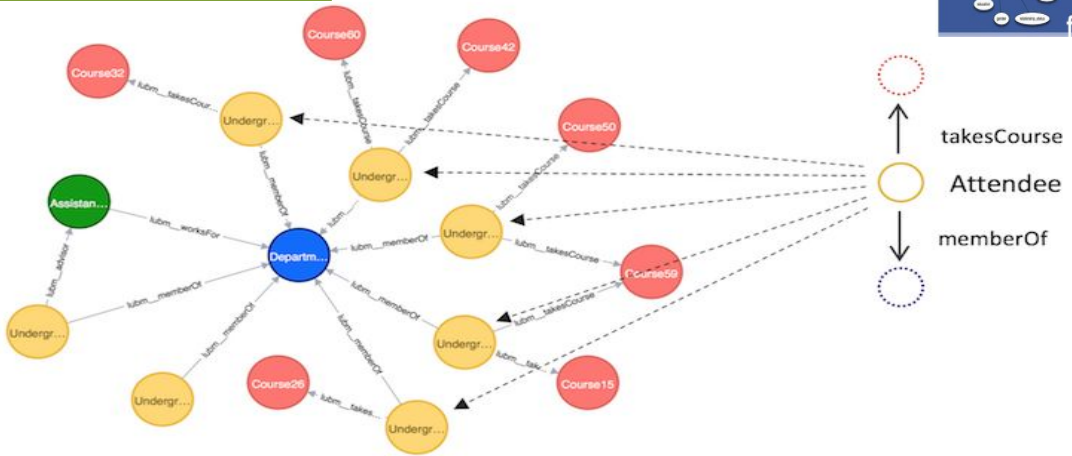
Humans:

- Explore data via intuitive/processible structure
- Combat information overload
- Tool for supporting knowledge-driven tasks

Also:

- Key ingredient for many AI tasks
- Bridge from data to human semantics
- Use decades of work on graph analysis



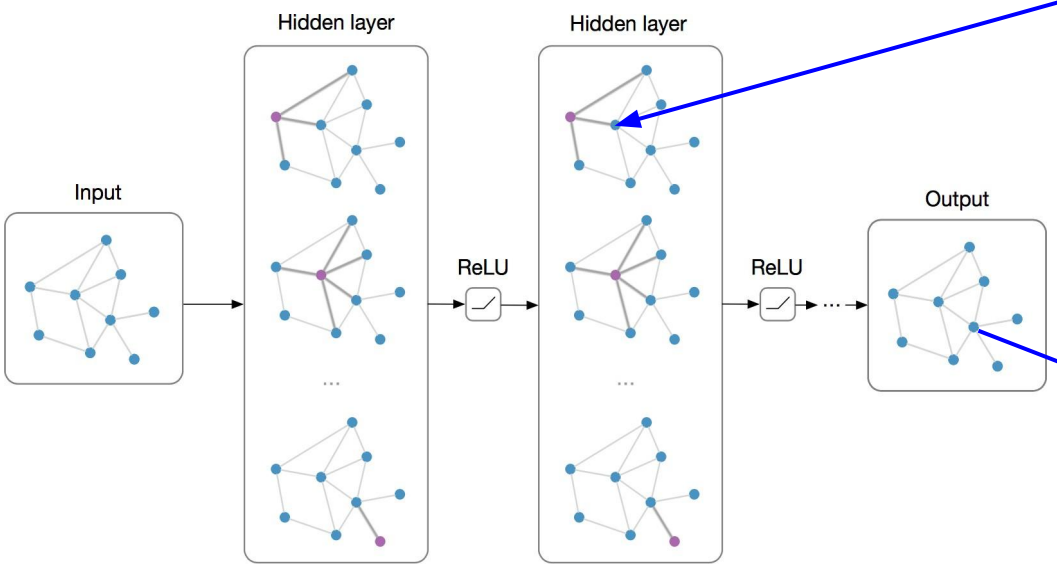


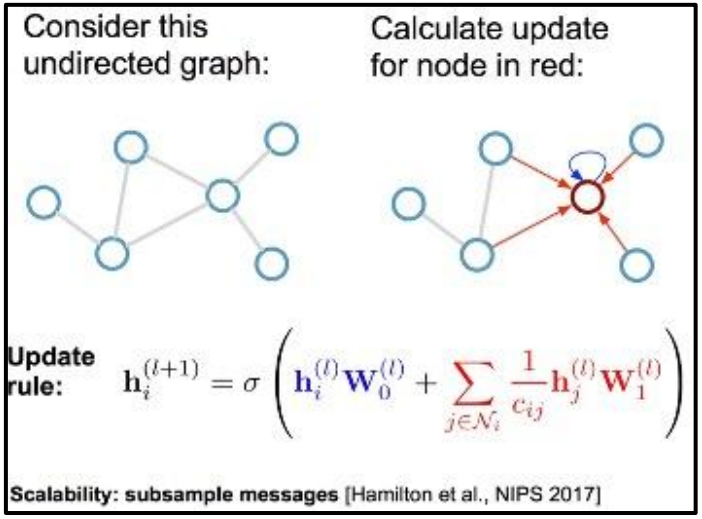
Graph Representation Learning: Enable Deep Learning on Graphs

Graph Neural Networks (GNNs)

Notation: $\mathcal{G} = (\mathbf{A}, \mathbf{X})$

- Adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$
- Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times F}$





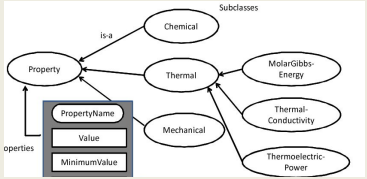
Downstream tasks:

- Node classification, link prediction…
- Graph classification, graph clustering…
- Anomaly detection, data imputation

Idea: Pass messages between nodes and agglomerate to refine node/edge representations

MDS^3-COE: A Knowledge Graph Learning Framework

Metadata, Ontologies
RDF triples, JSON
(abstraction/semantics/constraints)



... to data standardization & knowledge sharing

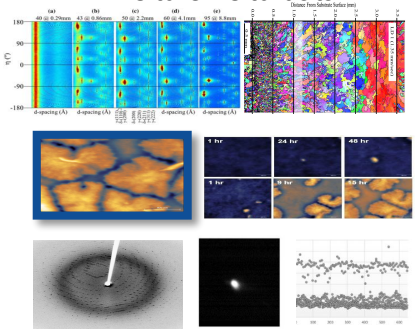
1 *validate* / *curate*

FAIRification

Featurization

2

Raw datasets
Image/videos, design data, in-situ/ex-situ data..



ML/AI models

physical con-straints

linked entities

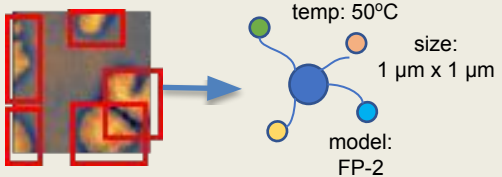
enriched features

Deep Learning

Summarization

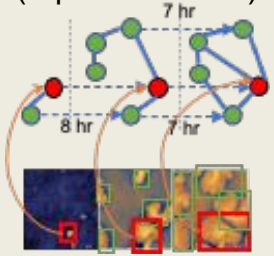
4 *cost-effective learning* / *efficient access & interpretation* **3**

Objects, Observations & Properties
(instances)



... to create AI/ML ready data resources

Scenes or st-Graphs
(representations)



Deep st-graph representation learning
... to inferential & predictive models

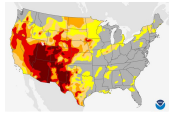
Summary Graphs
(patterns)

... to cost-effective data access, analysis & interactive exploration

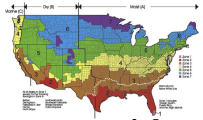
[1] Roger H. French et al., "Fairmaterials." The Python Package Index (PyPI), Oct. 08, 2021, https://pypi.org/project/fairmaterials/ .
[2] Willam C. Oltjen, et al., "FAIRmaterials: Make Materials Data FAIR." CRAN, Sep. 14, 2021, https://CRAN.R-project.org/package=FAIRmaterials .
[3] A. M. Karimi, et al., "Spatiotemporal Graph Neural Network for Performance Prediction of Photovoltaic Power Systems," in Proc. of AAAI,, 2021, https://ojs.aaai.org/index.php/AAAI/article/view/17799

Degradation Science with Spatiotemporal-Graph Models

image/satellite



climate/environment

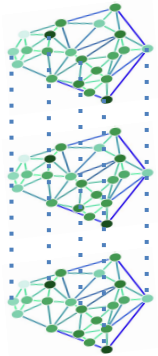


geospatial

featurizer

st-mapper

featurized network



time

querying/pattern mining

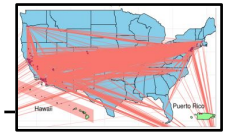
Metadata

Field & Lab Data

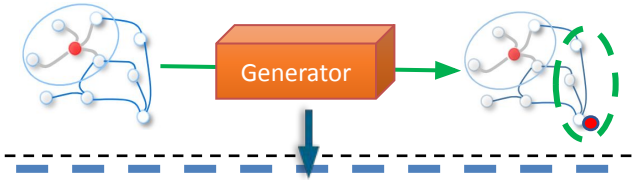
Manufacturing Data

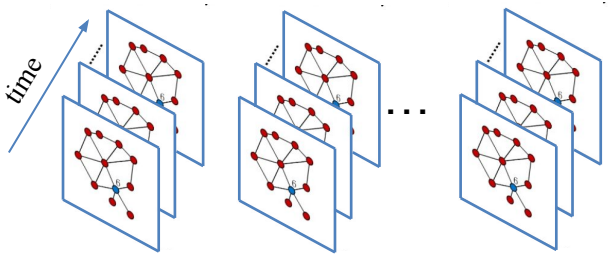
Material data storage: CRADLE

Domain/physical models & constraints



st-data augmentation





Graph Representation Learning:
message passing with spatiotemporal attention
in graph convolution layers, incorporating non-local
spatiotemporal dependencies

transform embeddings to downstream analysis

Classification

Clustering

Prediction/ forecasting

Decision making

Yinghui Wu, CWRU

[1] Chelsey Bryant, Nicholas R. Wheeler, Franz Rubel, and Roger H. French, “kgc: Koeppen-Geiger Climatic Zones.” The Comprehensive R Archive Network, Dec. 20, 2017 [Online]. Available: https://cran.r-project.org/package=kgc . [Accessed: May 24, 2021]
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[3] A. M. Karimi, B. G. Pierce, J. S. Fada, N. A. Parrilla, R. H. French, and J. L. Braid, “PVimage: Package for PV Image Analysis and Machine Learning Modeling.” May 08, 2020 [Online]. Available: https://pypi.org/project/pvimage/ . [Accessed: Feb. 28, 2020]
[4] Alan J. Curran, Tyler Burleyson, Sascha Lindig, David Moser, and Roger H. French, “PVplr: Performance Loss Rate Analysis Pipeline.” The Comprehensive R Archive Network, Oct. 07, 2020 [Online]. Available: https://CRAN.R-project.org/package=PVplr . [Accessed: Oct. 18, 2020]
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[8] Roger H. French et al., “Fairmaterials.” The Python Package Index (PyPI), Oct. 08, 2021 [Online]. Available: https://pypi.org/project/fairmaterials/
[9] Kris Zhao and Roger H. French, “hbspark: Package to pipe data from HBase to Spark (2+).” 2021 [Online]. Available: https://github.com/kxz167/hbspark . [Accessed: 29-Jan-2022]
[10] R. F.-0002-6162-0532) Huang(ORCID:0000-0003-0845-3293) Liangyi, “pointextract: Extract points information from 2d images to build a 3D object.” Jun-2022 [Online]. Available: https://pypi.org/project/pointextract/ . [Accessed: 22-Apr-2022]