PV Fleet st-Graph Neural Network Modeling:

Leveraging Spatiotemporal (st) Coherence, Distributed Computing, & Generative AI Models

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DOE-EERE-SETO Project: PV-stGNN Project: DE-EE0009353

CWRU UCF

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Materials Data Science for Stockpile Stewardship Center of Excellence

Traditional PV Performance Analysis

GS: Yangxin Fan[1], Raymond Wieser[1]

UG: Jiana Kambo[1], Hyangmok Baek[1]

Faculty: Yinghui Wu[1], Laura Bruckman[2], Roger H. French[1,2]

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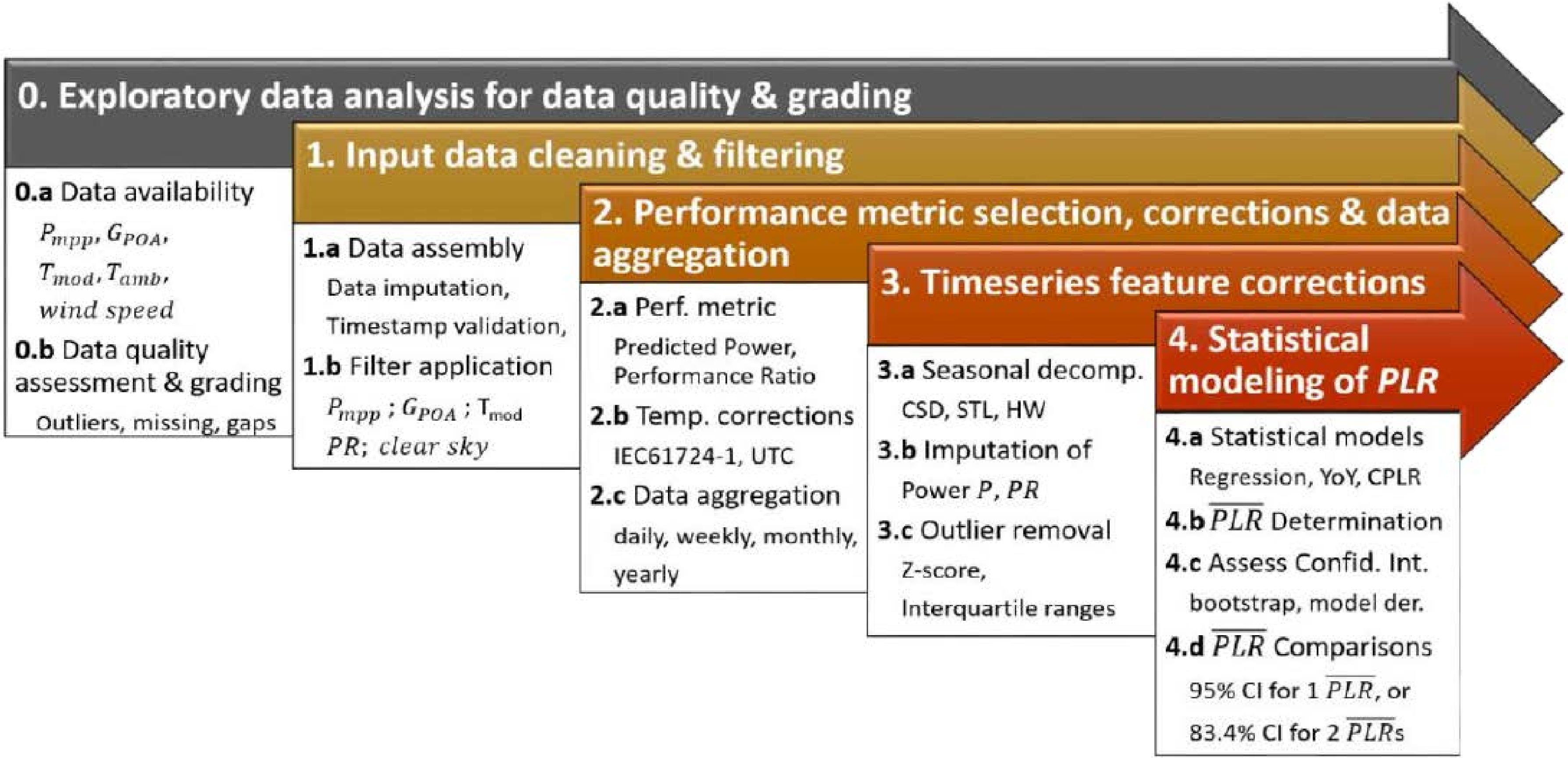
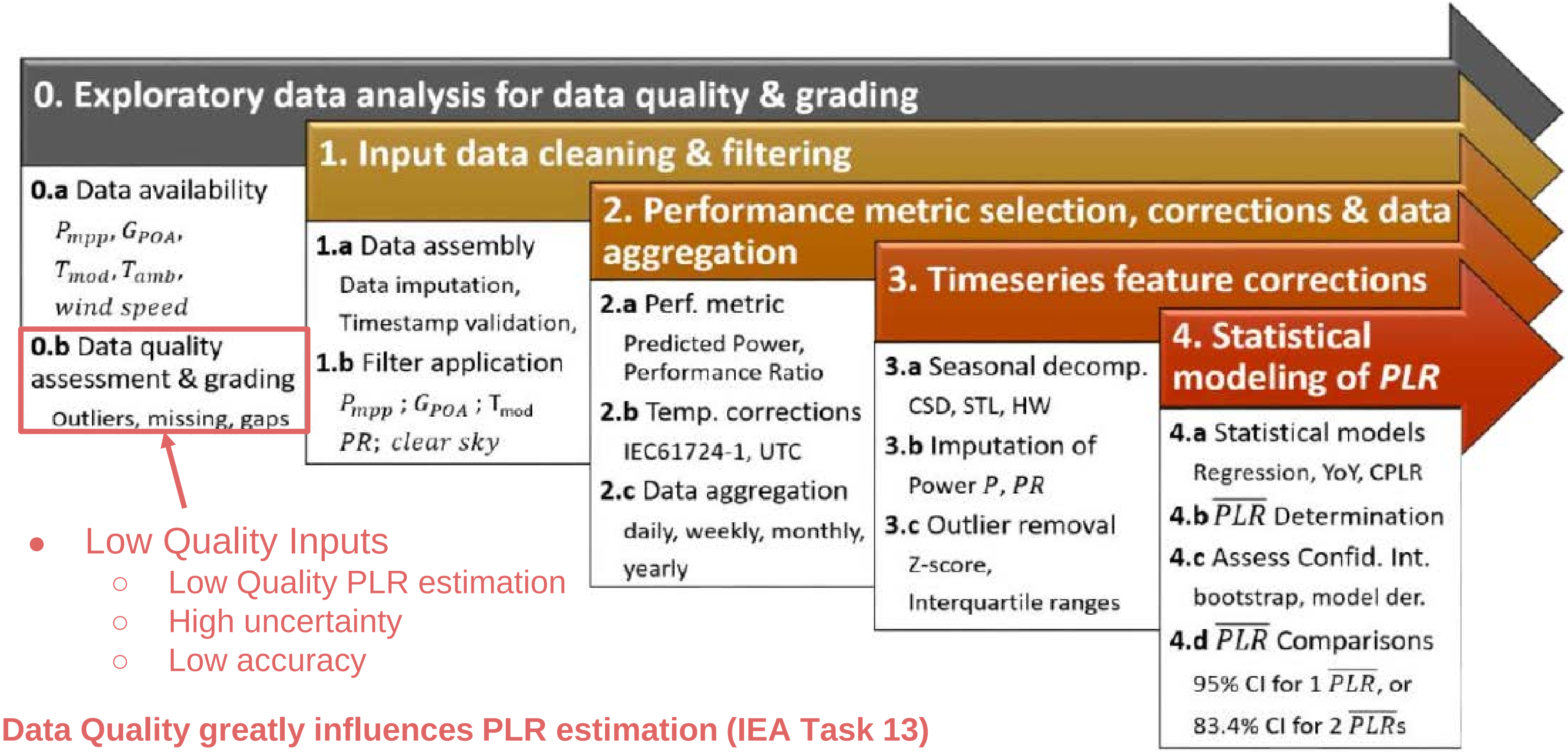
Award No: DE-EE0009353

Traditional PLR Estimation Framework: Five Steps: #0 to #4



R. H. French et al., "Assessment of Performance Loss Rate of PV Power Systems," IEA-PVPS, Task 13 Report, 2021.
[1] S. Lindig et al., "Intern.l collab. framework for the calculation of performance loss rates: Data quality, benchmarks, and trends (towards a uniform methodology)," Progress in PV, 29, 6, 673–602, Jun. 2021.

PLR Framework: Five Steps: #0 to #4, and how st-GNNs help?



- Low Quality Inputs
  - Low Quality PLR estimation
  - High uncertainty
  - Low accuracy

Data Quality greatly influences PLR estimation (IEA Task 13)

R. H. French et al., "Assessment of Performance Loss Rate of PV Power Systems," IEA-PVPS, Task 13 Report, 2021.
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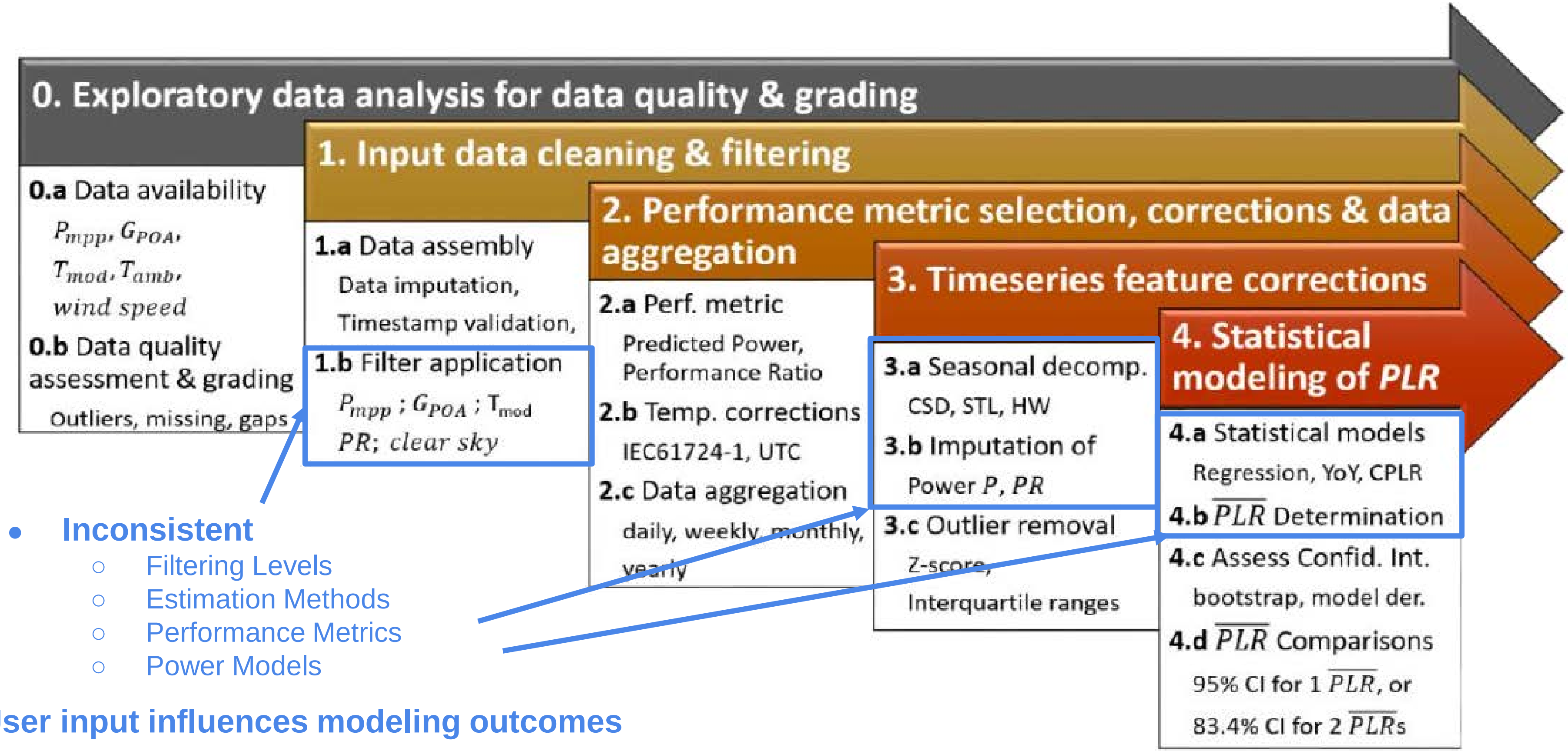

- **Inconsistent**
  - Filtering Levels
  - Estimation Methods
  - Performance Metrics
  - Power Models

User input influences modeling outcomes

R. H. French et al., "Assessment of Performance Loss Rate of PV Power Systems," IEA-PVPS, Task 13 Report, 2021.
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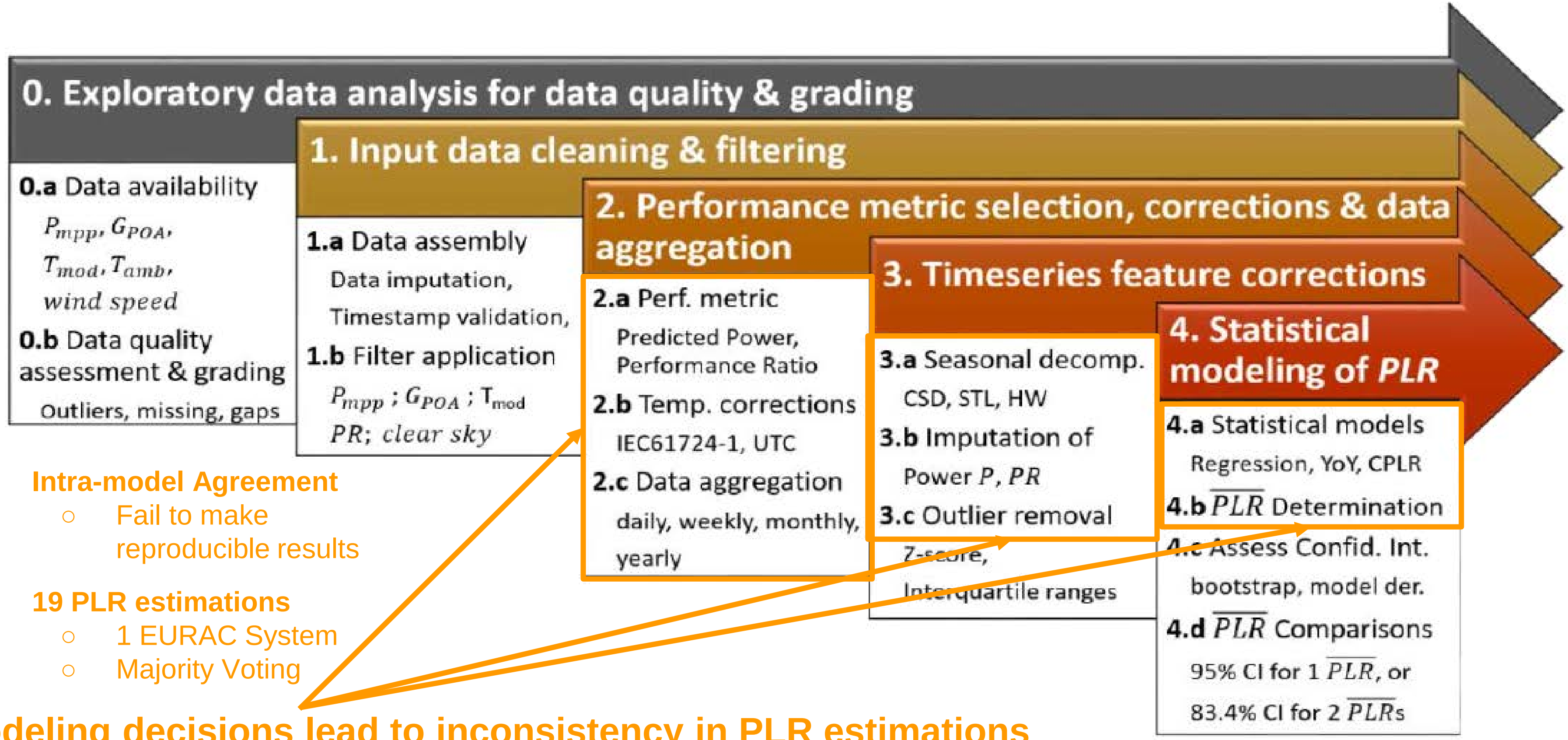

- **Intra-model Agreement**
  - Fail to make reproducible results
- **19 PLR estimations**
  - 1 EURAC System
  - Majority Voting

Modeling decisions lead to inconsistency in PLR estimations

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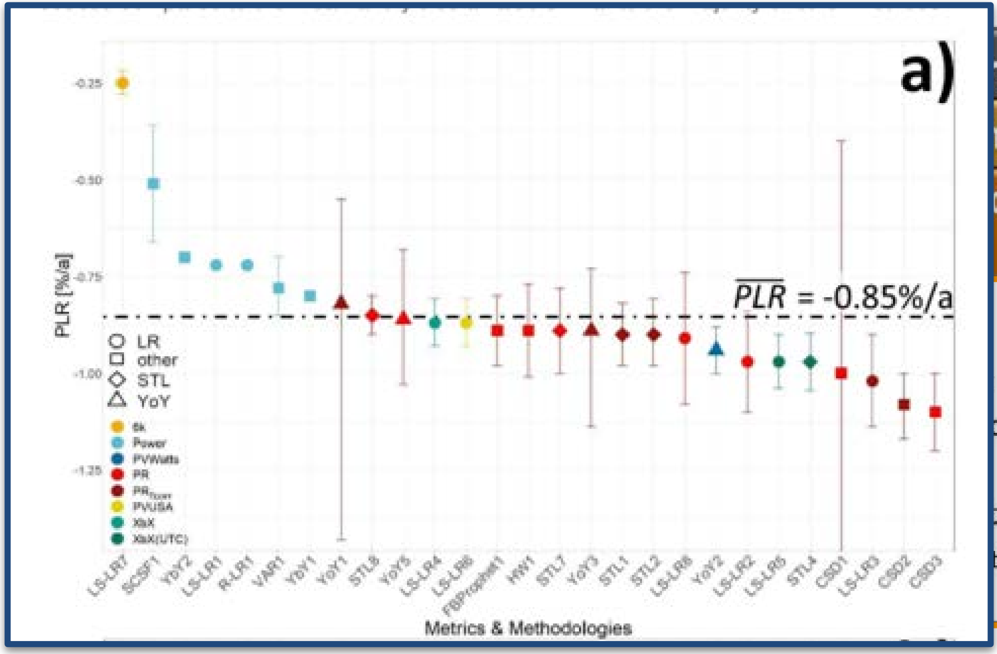

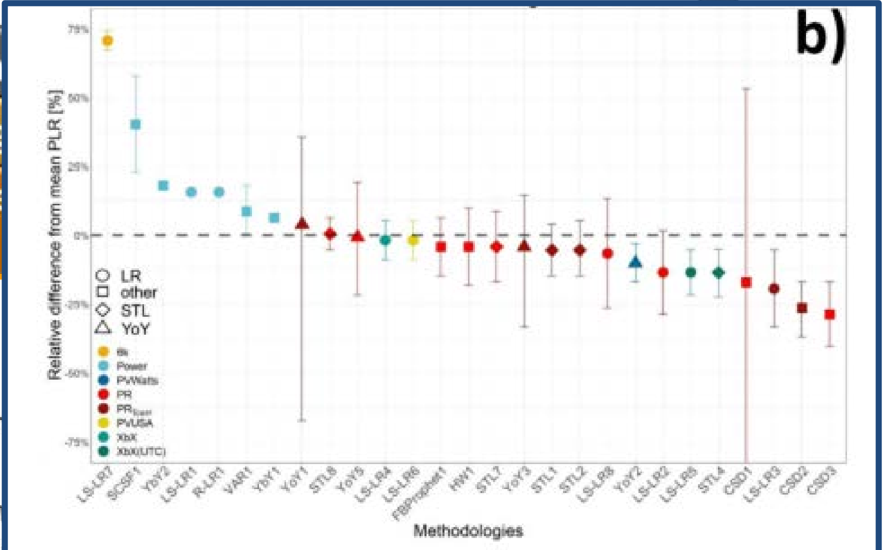

Figure 21: a) Calculated *PLR* of EURAC system; b) Relative calculated *PLR* values of EURAC system. The "error bars", are as reported by the analyst[1].
52

4.d $\overline{PLR}$ Comparisons

95% CI for 1 $\overline{PLR}$, or

83.4% CI for 2 $\overline{PLR}$s

Modeling decisions lead to

- inconsistency in PLR estimations

R. H. French et al., "Assessment of Performance Loss Rate of PV Power Systems," IEA-PVPS, Task 13 Report, 2021.
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Introduction to Graphs

Graphs are data structures that represent a

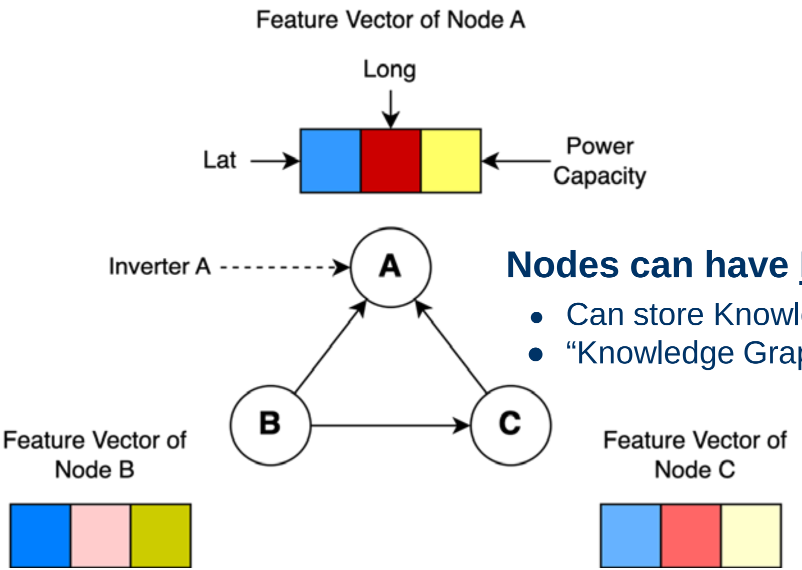
- set of objects (**nodes**) that are **connected**
- by some type of relationship **(edges)**

Distinct Objects ("Nodes")

- Represent an entity
  - E.g,: a traffic sensor, a PV inverter, etc.
- Can hold multiple types of information
  - In their "feature vectors",
- This nodal information can be either
  - **Static** (such as in a knowledge graph)
    - Constant properties of nodes
  - **Time-varying**
    - Timeseries (discrete or continuous)
      - Power, Weather, Irradiance

Relationships ("Edges")

- Edges can have **directions**
  - Undirected or Directed
    - Undirected: (A → B) = (B → A)
    - Directed: (A → B) ≠ (B → A)



Nodes can have Feature Vectors

- Can store Knowledge
- "Knowledge Graph" repositories

Example of a featurized PV Graph (3 inverters)

What are Spatiotemporal Graphs (st-graph)

st-graphs are special type of graphs

Where nodes contain

- **Time-varying feature vectors**
  - Single-channel: one timeseries per node
  - Multi-channels: multiple timeseries per node

$$W_{i,j} = \begin{cases} \exp\left(-\frac{d_{ij}^2}{\sigma^2}\right), i \neq j \text{ and } \exp\left(-\frac{d_{ij}^2}{\sigma^2}\right) \geq \epsilon \\ 0 \text{ otherwise} \end{cases}$$

ε-thresholded Gaussian Kernels, control graph sparsity

ε : spatial coherence,

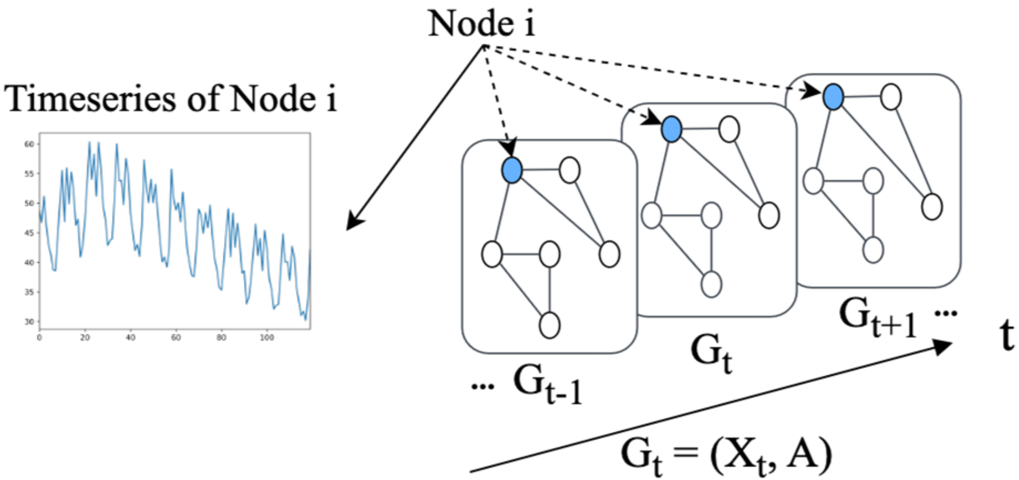
distanced-based threshold

- Between 0 and 1
- Controls the sparsity of graphs
  - When **ε** = 0, all nodes connected with each other
  - When **ε** = 1, all nodes isolated, unconnected

Spatiotemporal graphs

denoted as $G_t = (X_t, A)$

- X_t: the time-varying node features
- A: static adjacency matrix



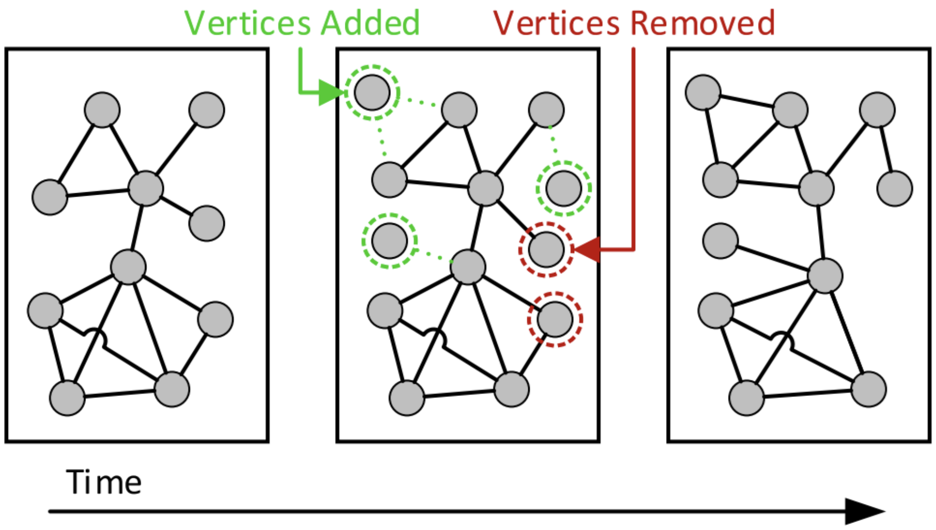
Spatiotemporal Graphs with Single-channel Feature Vectors

What are Dynamic Graphs

Mathematically, dynamic graphs are

defined as $G_t = (X_t, A_t)$

- X_t : the time-varying node features
- A_t : dynamic adjacency matrix,
  - captures dynamic changes in connections
  - between of nodes over time
- **So dynamic graphs enable Generative AI**
  - Through Node Addition
  - And Node Removal



Dynamic graphs (graph structures vary with time)[1]

Previously, we defined the st-graph as

$$G_t = (X_t, A)$$

- Hence st-graph can be seen as
- A dynamic graph with static graph structure

Spatiotemporal-Graph (st-Graph) Learning:

Timeseries Imputation

& Trend Estimation

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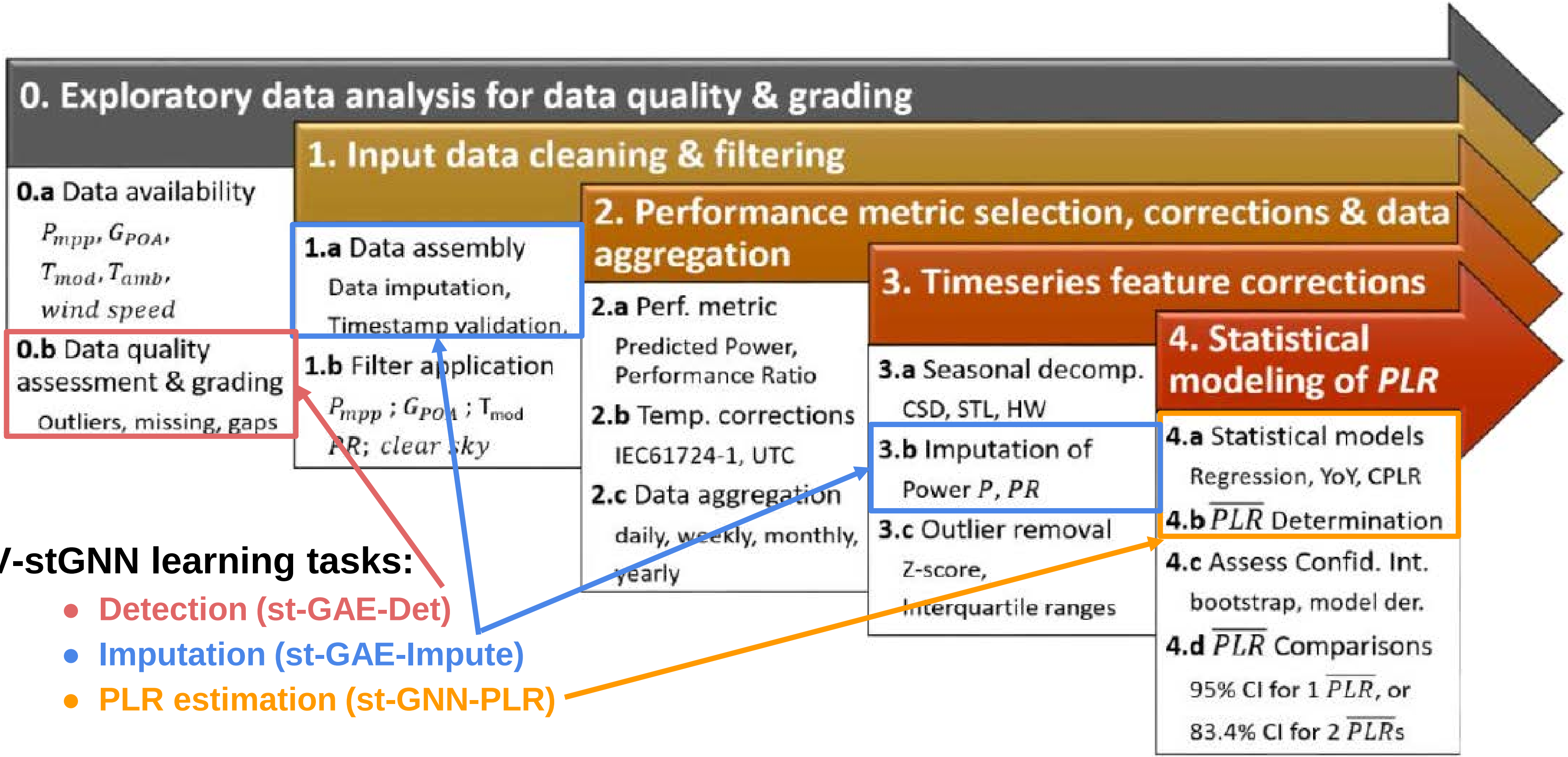
[1] A. M. Karimi, Y. Wu, M. Koyuturk, and R. H. French, "Spatiotemporal Graph Neural Network for Performance Prediction of Photovoltaic Power Systems," in Proc. AAAI Conf. on Art. Intel., May 2021, 8.

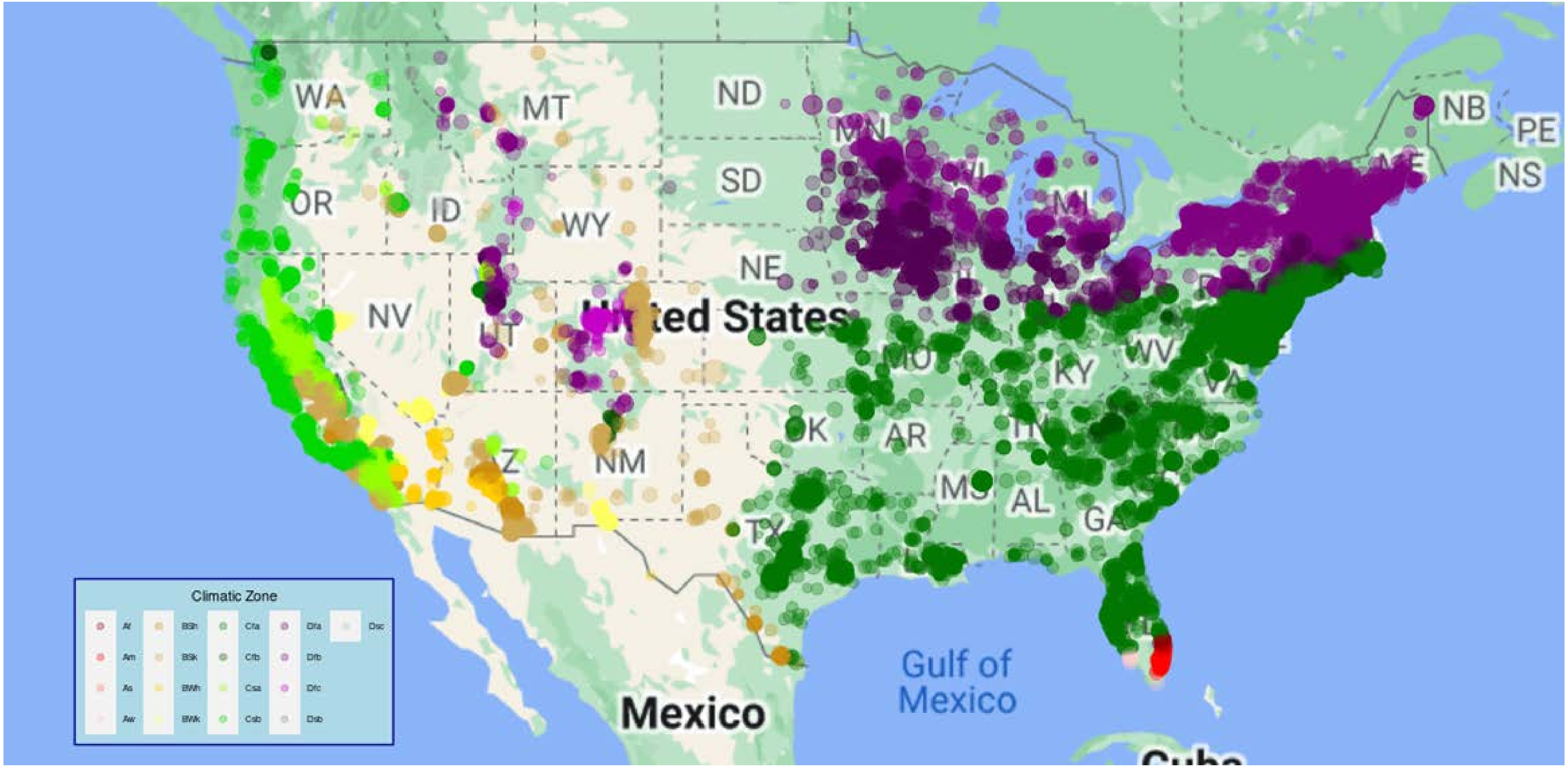
PLR Framework: Five Steps: #0 to #4, and how st-GNNs help?



PV-stGNN learning tasks:

- Detection (st-GAE-Det)
- Imputation (st-GAE-Impute)
- PLR estimation (st-GNN-PLR)

Large Scale Photovoltaic Fleet Monitoring: 104,700 PV Systems



CRADLE Data Explorer: PV Systems, {meta}data, Quality

Ingest 100,470

Photovoltaic Systems

- To CRADLE3
  - Into HDFS
  - As Parquet Files
- Using **Apache Spark3**

Distributed Across

- 1000 CPUs
- 100 HDDs

Apache Impala

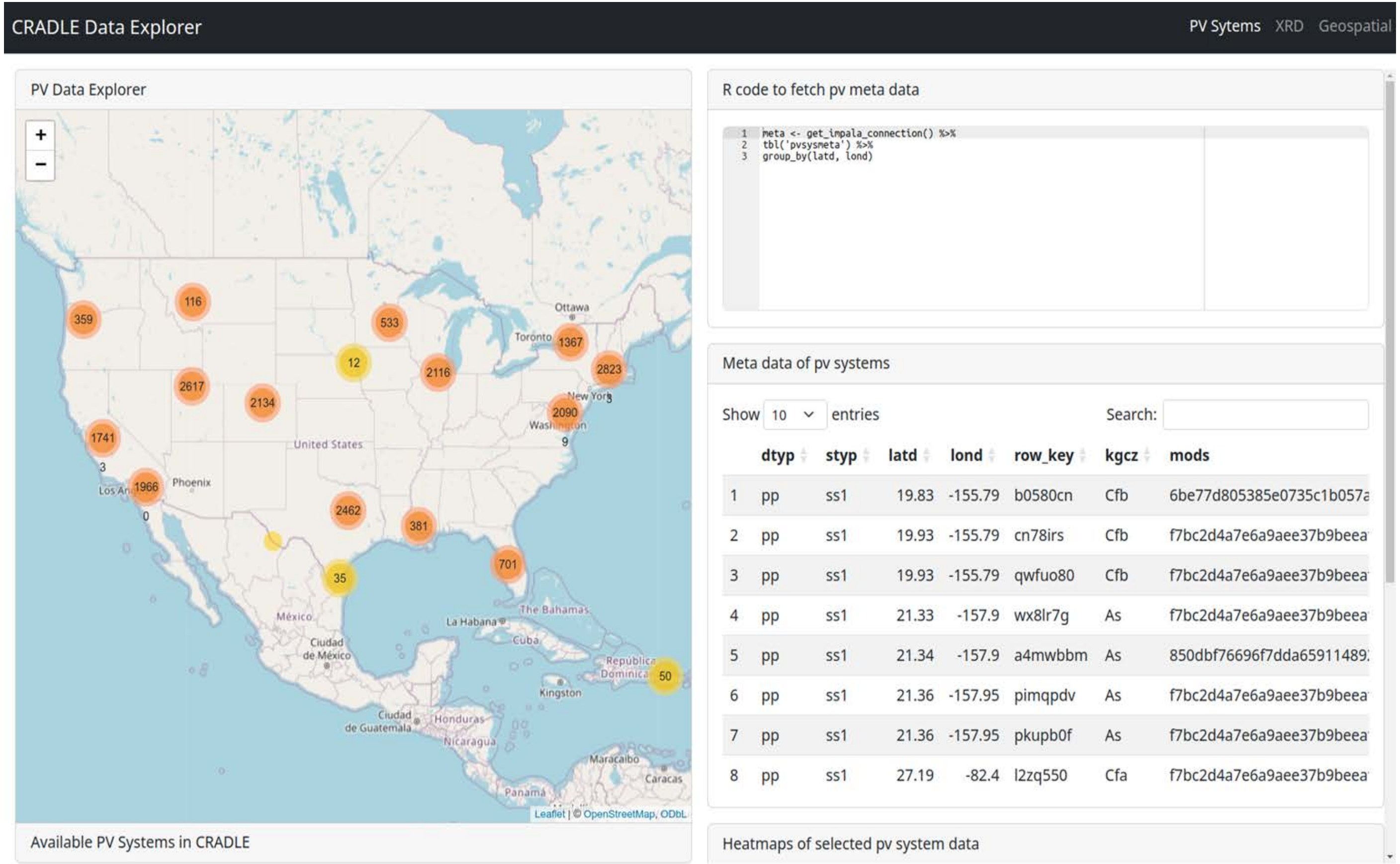
- For SQL Queries

Provide Codebox

- For Customized Queries

Retrieve All Metadata

- Data Quality Heatmap

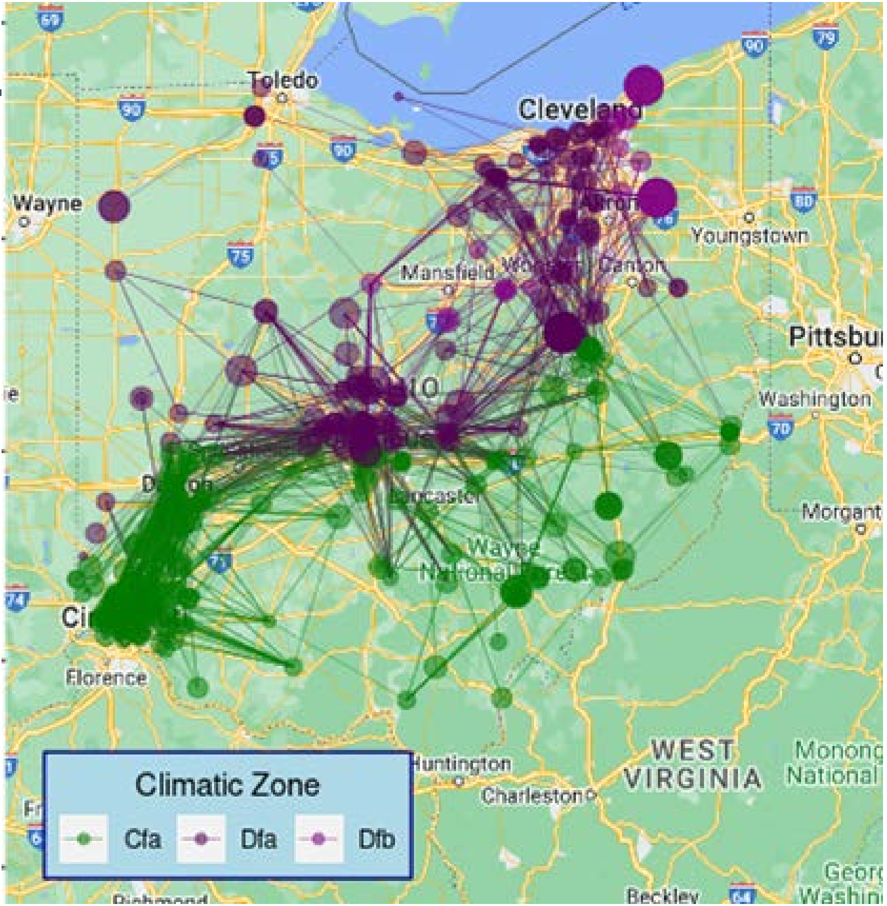


PV Network Representation

Inverters
- “Nodes”
- Individual Timeseries

Site “Similarity”
- “Edges”
  - How much information
  - Should connections “share”

Evaluating “Similarity”
- Distance (Spatial Coherence)
- Cell Type
- Nameplate Power
- Benefits from “FAIRified” datastreams



Network Representation of 295 Inverters
(edges sparsified for visualization)

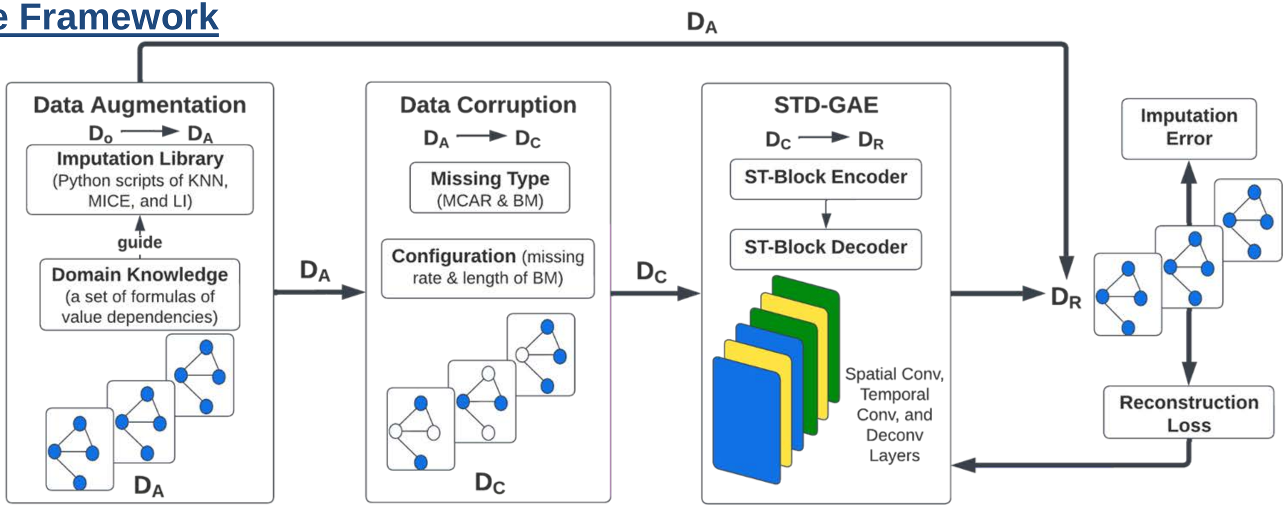
Timeseries Data Reconstruction, & Generative Data Imputation

For PV: Performance Loss Rate (PLR)
- Critical to profitability of asset

Data Quality Impacts PLR estimates
- Low Quality Data
  - Low Quality PLR estimation
  - High uncertainty, Low accuracy

Data Imputation improves low quality data
- Physical Models
- Predictive Mean Matching
- Gradient Boosting Regression
- Traditional Imputation Methods

The stGAE-Impute Framework



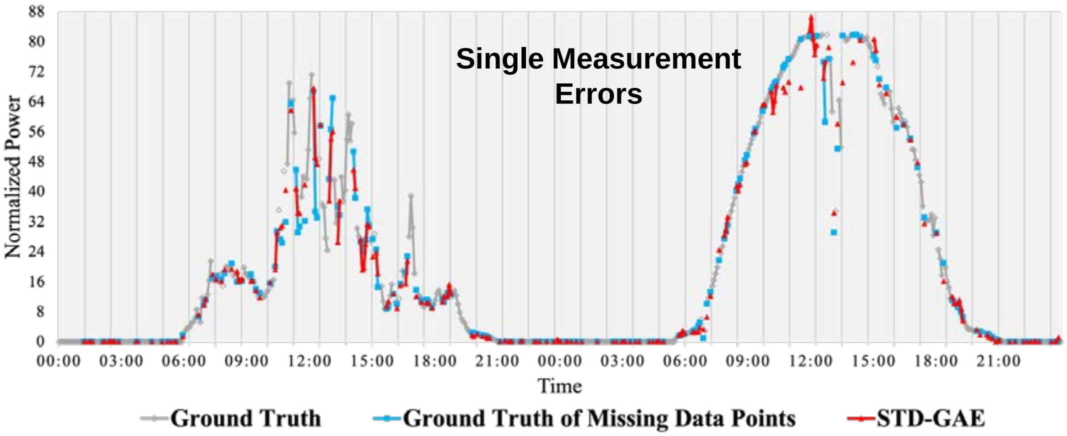
D_A: Augmented PV Data; D_C: Corrupted PV Data; D_R: Recovered PV Data.

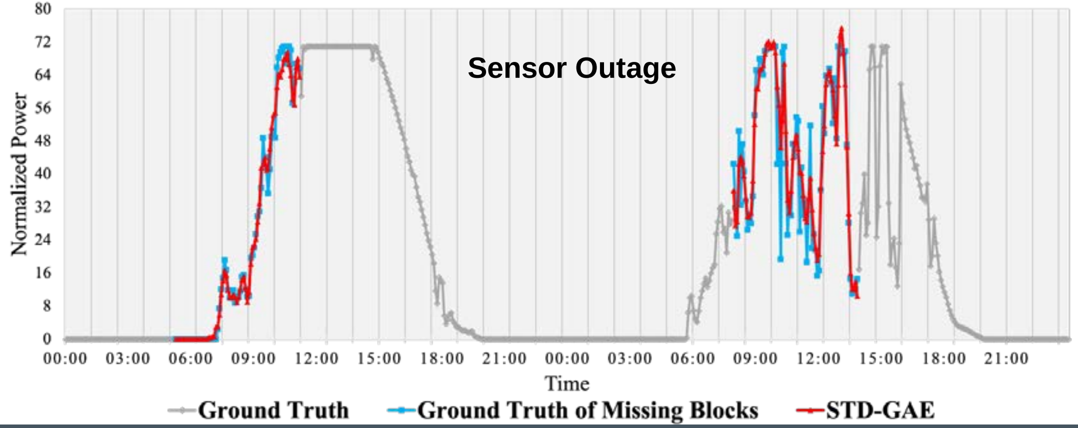
[1] Y. Fan, X. Yu, R. Wieser, … L. Bruckman, R. French, Y. Wu, "Spatio-Temporal Denoising Graph Autoencoders with Data Augmentation for Photovoltaic Data Imputation," in Proc. ACM on Management of Data, 2023, 1, 1–19.

Data Imputation Accuracy

st-GAE

- Missingness Types
  - Single Value Corruption
  - Measurement Outage
- Missingness Severity
  - 10% - 60% Measurements Missing
  - 2hrs - 6hrs Inverter Outage



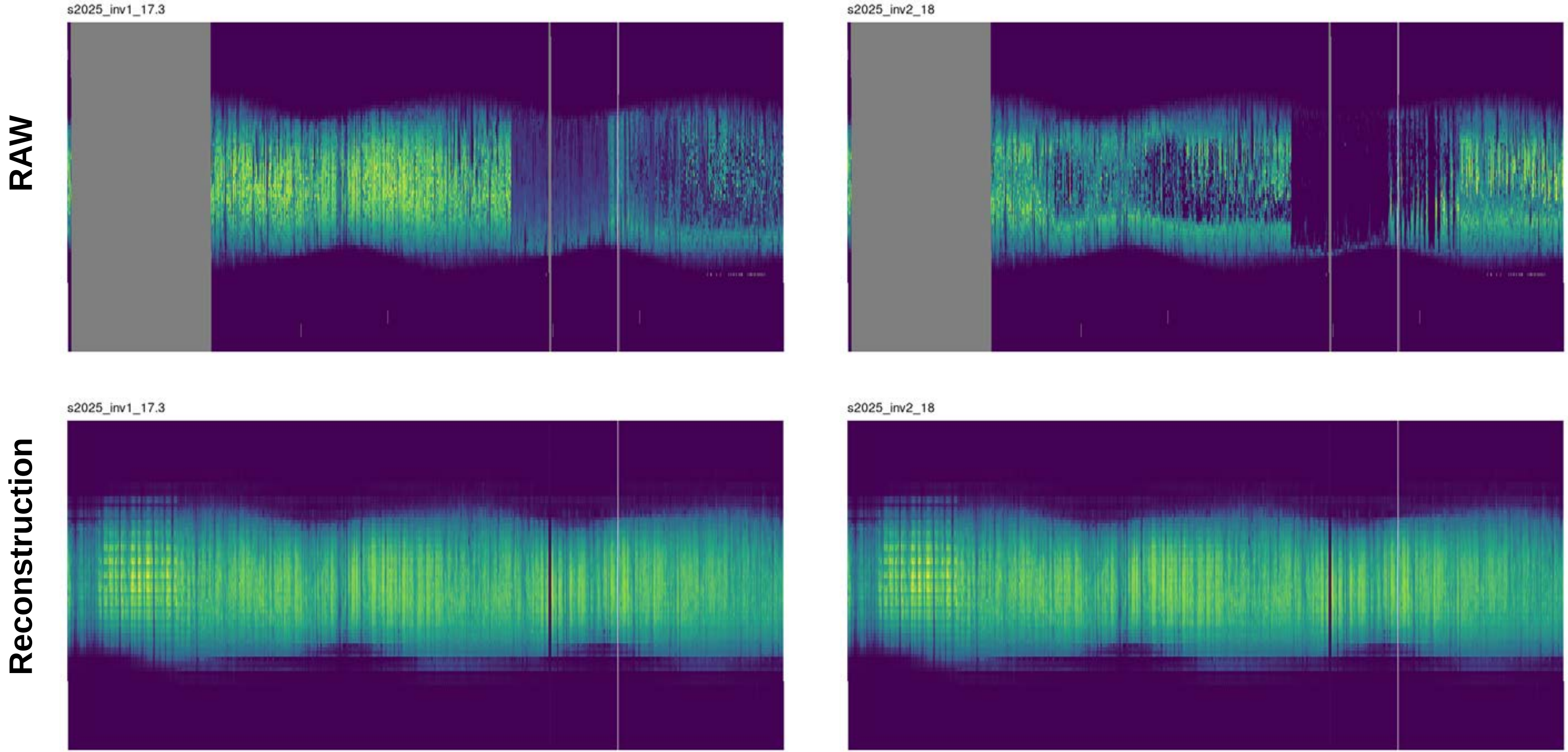


Model Accuracy

- Insensitive
  - Missingness Types
  - Missingness Severity
- st-GAE Outperforms
  - Traditional
  - Deep Learning

[1] Y. Fan, X. Yu, R. Wieser, … L. Bruckman, R. French, Y. Wu, "Spatio-Temporal Denoising Graph Autoencoders with Data Augmentation for Photovoltaic Data Imputation," in Proc. ACM on Management of Data, 2023, 1, 1–19.

Data Reconstruction: Block Outages & Anomalous Measurements



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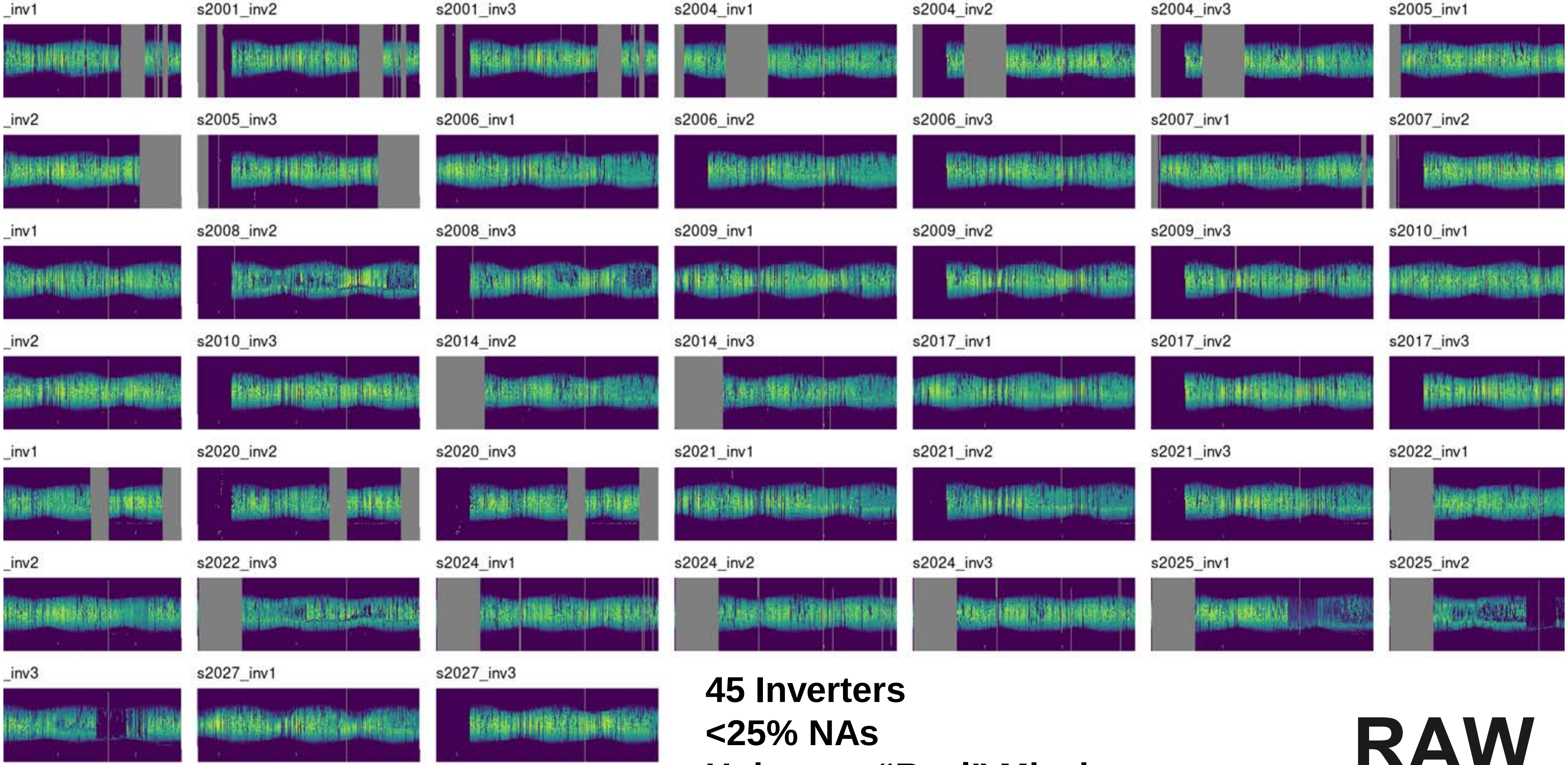
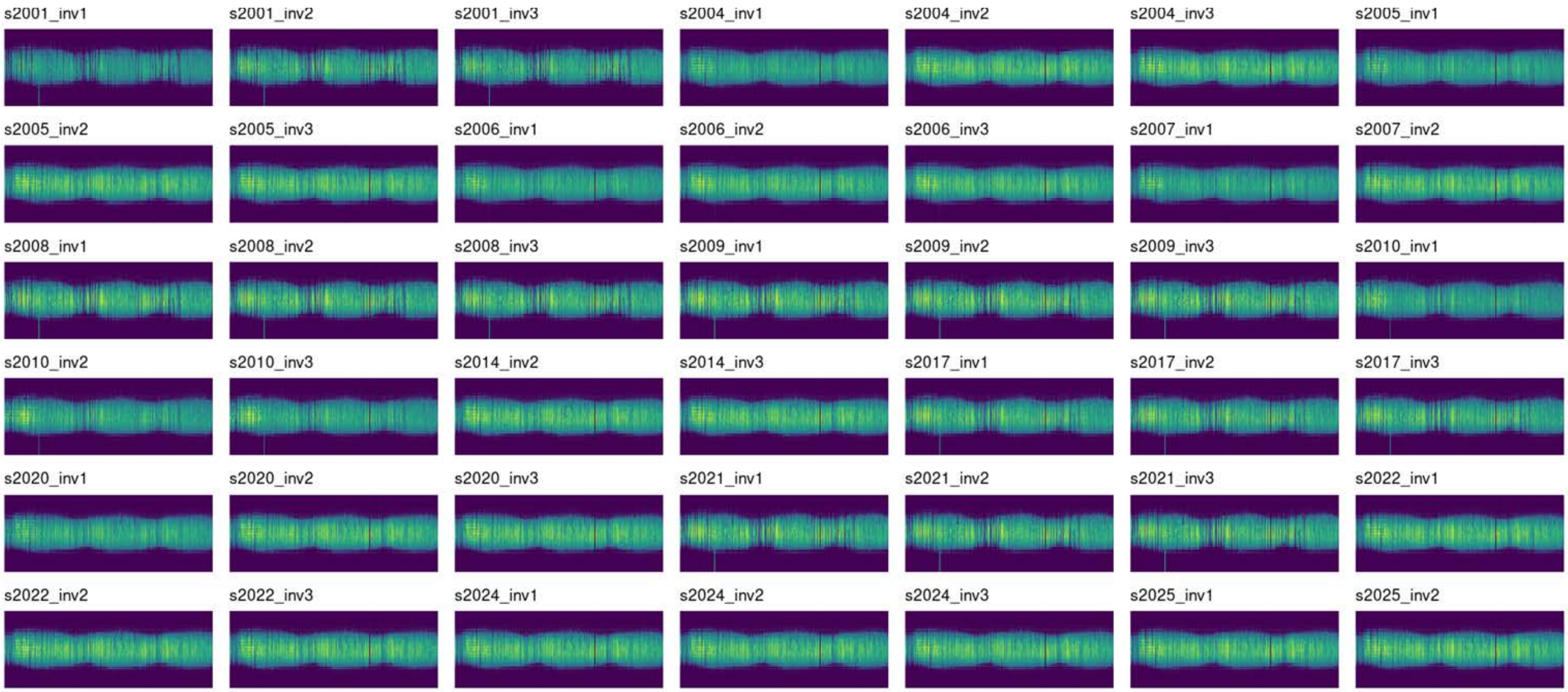
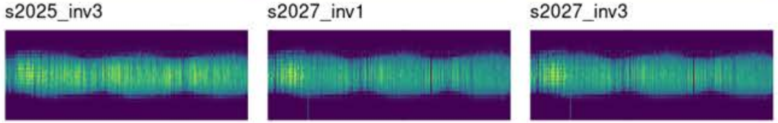


45 Inverters
<25% NAs
Unknown "Real" Missingness

RAW





45 Inverter **“Reconstruction”**

Spatial - Temporal Imputation

0% Missingness

st-GAE

Motivation of PV-stGNN-PLR

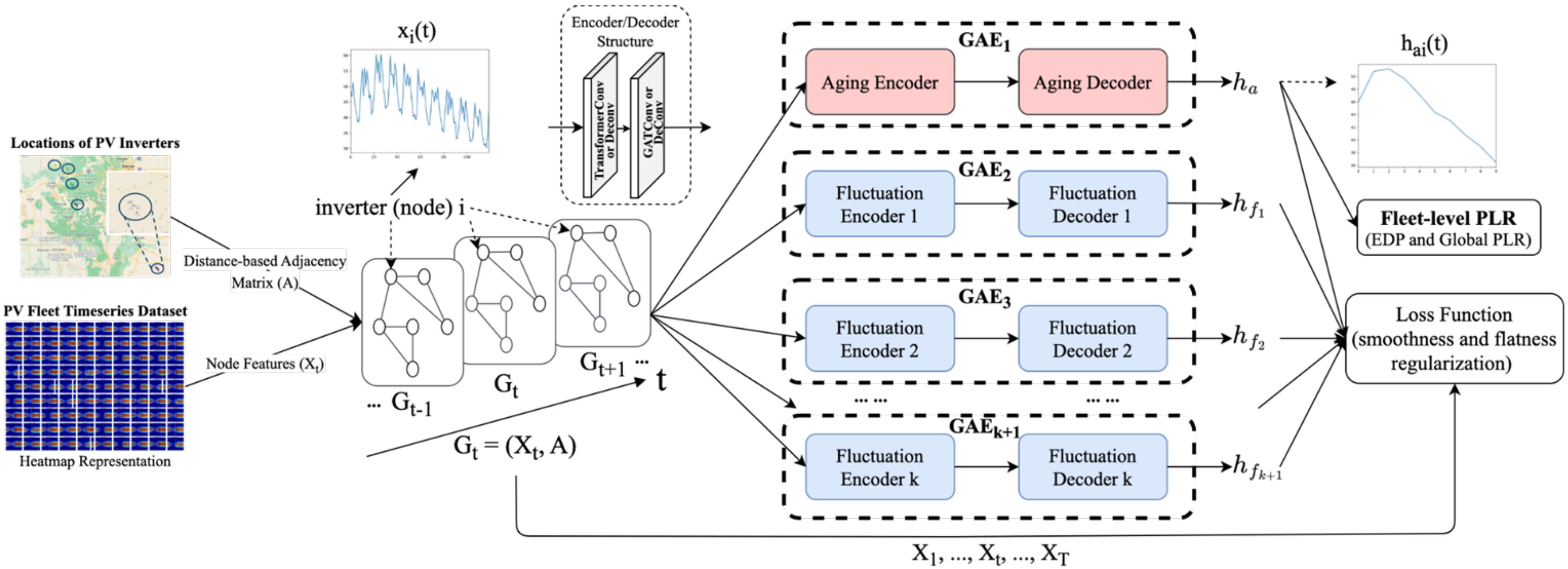
Traditional PLR estimation methods face following challenges:

- Lack of reproducibility: PLR may be straightforward, the pipelines are complex
  - requires domain-knowledge guided decisions
- Data Quality: missing or erroneous data can occur
  - adds complexity and uncertainty to the results
- Non-linearity: a single PLR value cannot characterize non-linear PLR degradation patterns

PV-stGNN-PLR addresses above challenges through:

- A light-weighted spatio-temporal graph neural network-based model
  - Utilizes spatio-temporal coherence within PV fleets
- A novel loss function
  - to ensure clear disentanglement between extracted aging and fluctuation
- Automated Data Preprocessing
  - st-GAE imputation improves data quality

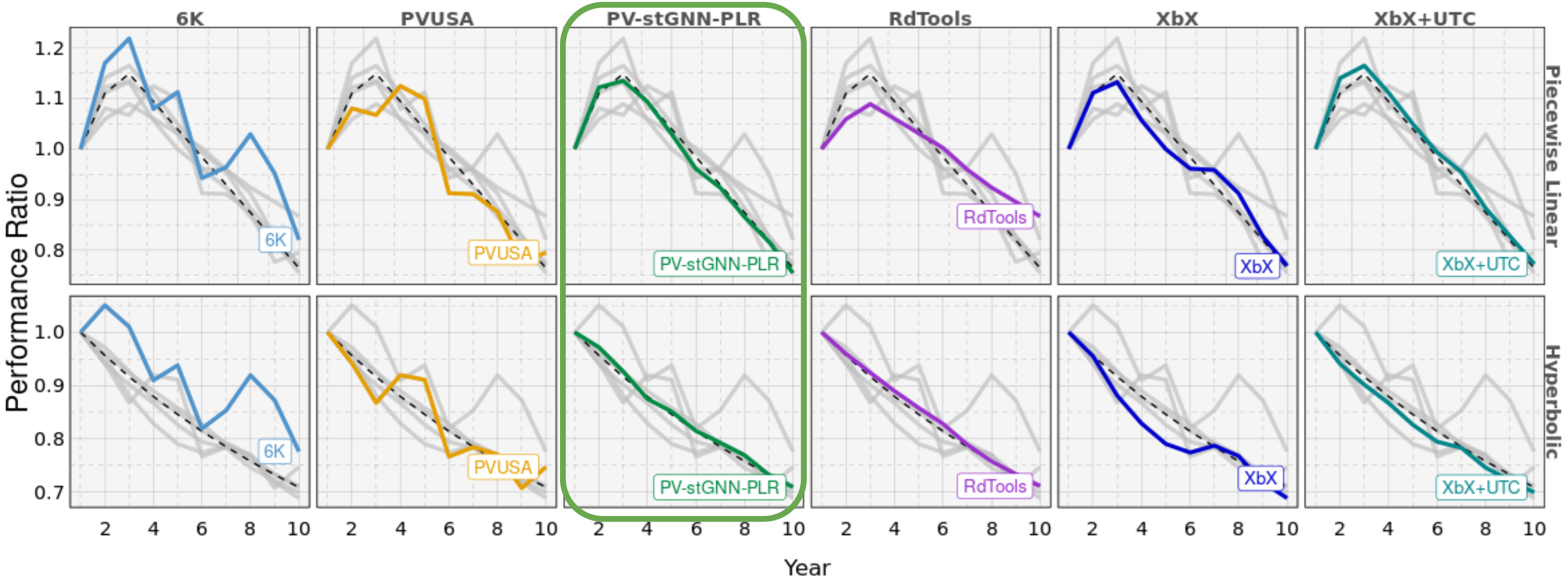
Timeseries Decomposition Framework: For PLR Determination



- **"Parallel-friendly" K+1 GAE (graph autoencoder) blocks**
- **One aging-term**
  - Extracts the long-term degradation pattern for PLR analysis
- **K different fluctuation terms**
  - Captures seasonalities and noises at different temporal resolutions

[1] Y. Fan, R. Wieser, X. Yu, J. Braid, A. Shaton, A. Hoffman, T. Didier, B. Spurgeon, D. Gibbons, L. S. Bruckman, Y. Wu, and R. H. French, "Using Neural Network Decomposition to Estimate Field Photovoltaic Performance Loss Rate," presented at the IEEE PVSC 50, San Juan Puerto Rico USA, 2023.

Trend Decomposition and Extraction



We compare **Estimated Degradation Pattern (EDP)** extracted by PV-st-GNN-PLR
With top six best-performed baselines with **Real Degradation Pattern (RDP).**

- PV-st-GNN-PLR can better recover real degradation pattern
- EDP extracted by PV-st-GNN-PLR is the closest to RDP
  - in both Piecewise Linear and Hyperbolic degradation patterns
  - followed by XbX+UTC and RdTools (Hyperbolic)

CRADLE Computing

GS: Arafath Nihar[1], Olatunde Akanbi[1], Tommy Ciardi[1], Tian Wang[1]
UG: Rachel Yamamoto[1], Rounak Chawla[1], Hayden Caldwell[1],
Faculty: Yinghui Wu[1], Vipin Chaudhary[1], Roger H. French[1,2]

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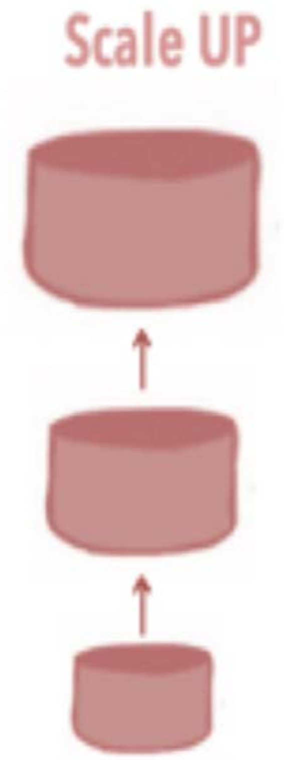
CRADLE Hardware: HPC Scaling up



Pioneer HPC: 5912 cores
- 32 gpu nodes

Markov HPC: 1240 cores
- 16 gpu nodes

One Compute Node
- Up to 40 cores
- Up to 1Tb RAM memory
- Nvidia v100
- Up to 32 GB of GPU VRAM

HPC Compute Model
- Lots of FLOPS
- But Limited, Expensive Data Storage

CRADLE Hardware: HPC Scaling up

Nvidia AISC: 32 integrated GPU nodes

- 4 Nvidia DGX Pods, of 8 A100 GPUs
- 2.56 Tb GPU VRAM
- 4 Tb of RAM memory
- 15 Tb NVME storage

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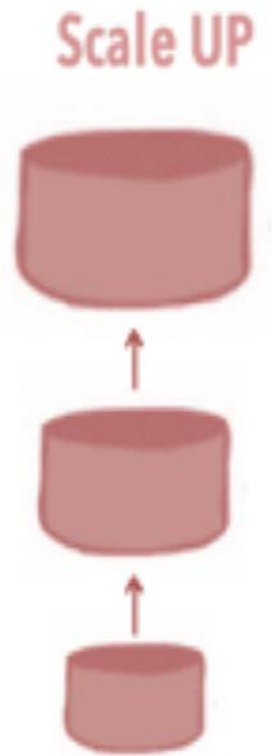

CRADLE Hardware: Distributed Hadoop Scaling Out, for CRADLE 3.2

4 Name Nodes

- 224 Cores
- 2 Tb of RAM memory
- 21.6 Tb Storage

15 Data Nodes

- 840 Cores
- 3.84 Tb of RAM memory
- 1.92 Pb of Storage TB
- 30 NVIDIA Ampere A2 GPU

= 1.95 Pb of storage

CRADLE D/HPC

- Dist. Compute
  - 2.5 Pb Cluster
  - 7 TB Ram
  - 1164 CPU Cores
  - 30 GPUs
    - 480 GPU VRAM
    - 384k Cuda Cores
    - 1.2k Tensor Cores
- High Perf. Compute
  - 7152 CPU Cores
- Nvidia AISC 8-DGX
  - 2.5 Tb VRAM
  - 4 Tb RAM
  - 15 Tb nvme storage

Large st-Graph Calculation Benchmarks

Benchmark tests using CRADLE's

- State-of-the-art CPUs & GPUs

Compute 100K^2 adjacency matrix

- Using multi-processing per compute node
- And fleet out jobs across compute nodes
  - Using SDLEfleets package:
    - ~19 Days ➞ ~ 2 hrs

Use 1 NVIDIA A100 GPU, 80GB VRAM

- For large-scale graph learning
  - Without subgraph sampling

AISC is 32 Integrated A100 GPUs!

- With integrated RAM & NVME Storage
- A critical form of Compute Integration

Benchmark Results

- **Model: st-GAE-Impute**
- **Large Scale st-Graph AutoEncoder**
  - 10k nodes, ~1 million edges
  - 1-year timeseries for each node
  - 5-minutes interval
- **Training time**
  - Using 1 year of timeseries data
    - 5 min. Interval
  - Run time: 1 hour 55 minutes
    - Epsilon = 0.25
- **Inference time: For Data Imputation**
  - On two-months data
  - Run time: 56 seconds

PV System Analytics:
Dynamic Graphs
&
Graph Generative AI

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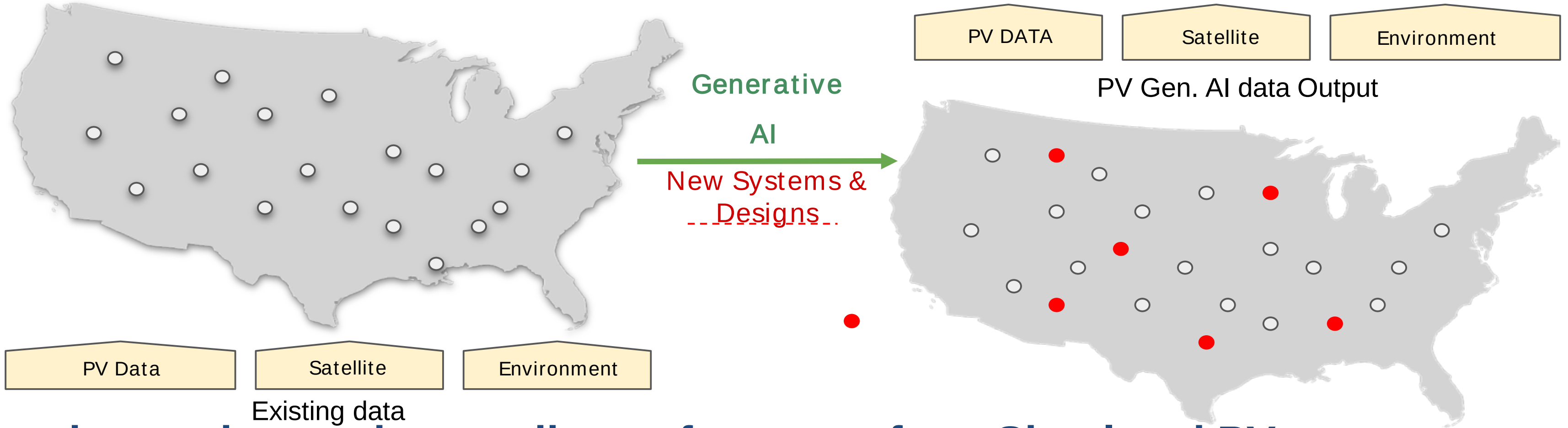
PV System Modeling / Prediction

AI Generated Virtual PV System Performance



Graphs can be used to predict performance for a Simulated PV system

st-GNNs are a type of "Data-driven Digital Twin"

- Leverage existing systems' datastreams to learn

Can Generate & Predict performance of new Virtual PV Systems

- From Dynamic Graph's Imputed Node Features
  - Power / Meteorology / System Info

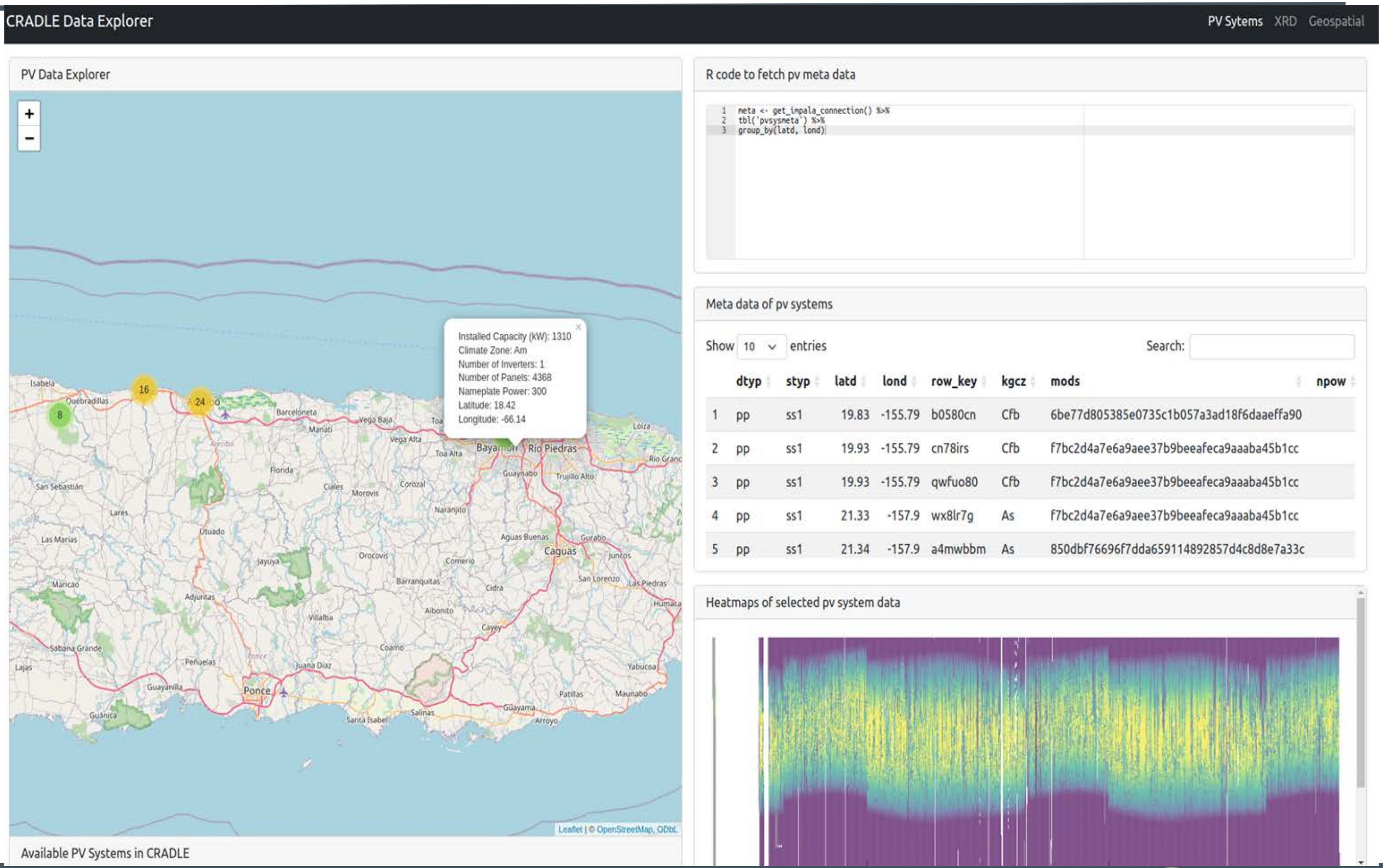
How do Dynamic Graphs Enable Generative AI?

Graph learning for PV

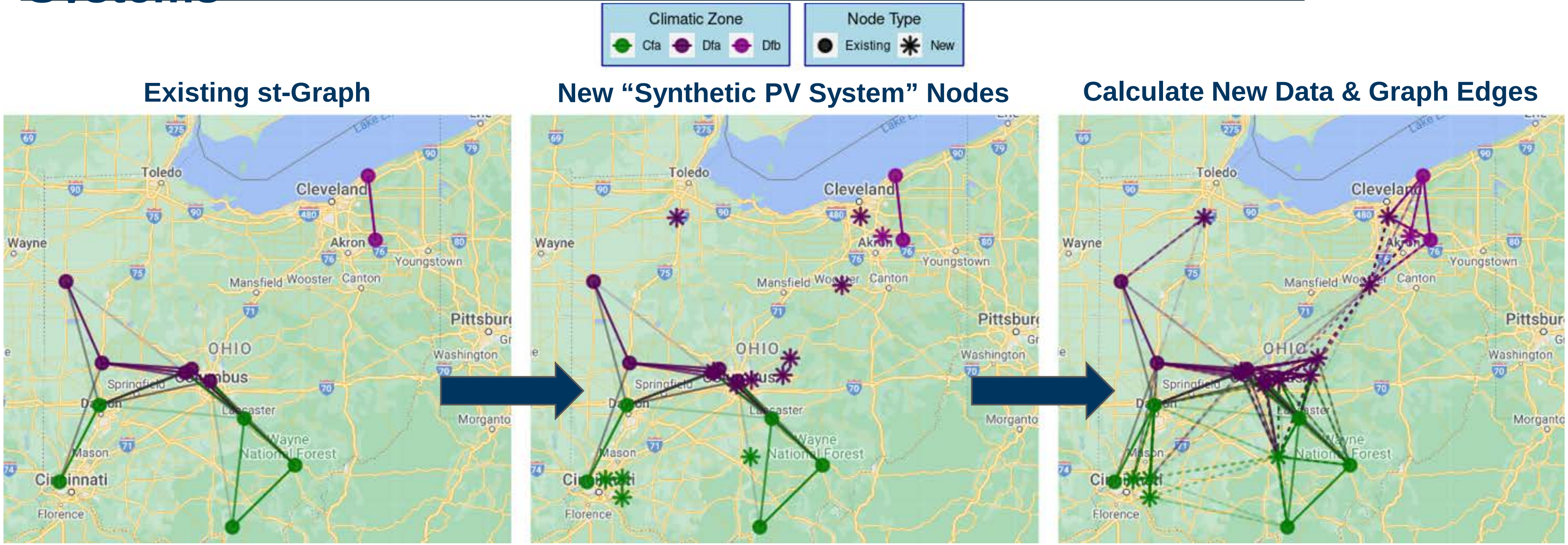
- Node features represent
  - PV system properties

Node features Include

- **Static Features**
  - Time invariant attributes (constants)
    - Installed Capacity
    - Climate Zone
    - Model Type
- **Dynamic Features**
  - Timeseries (time-varying)
    - Meteorological Data
      - Temp. Wind, Irrad. etc.
    - Power Output
    - IV - Curve Traces



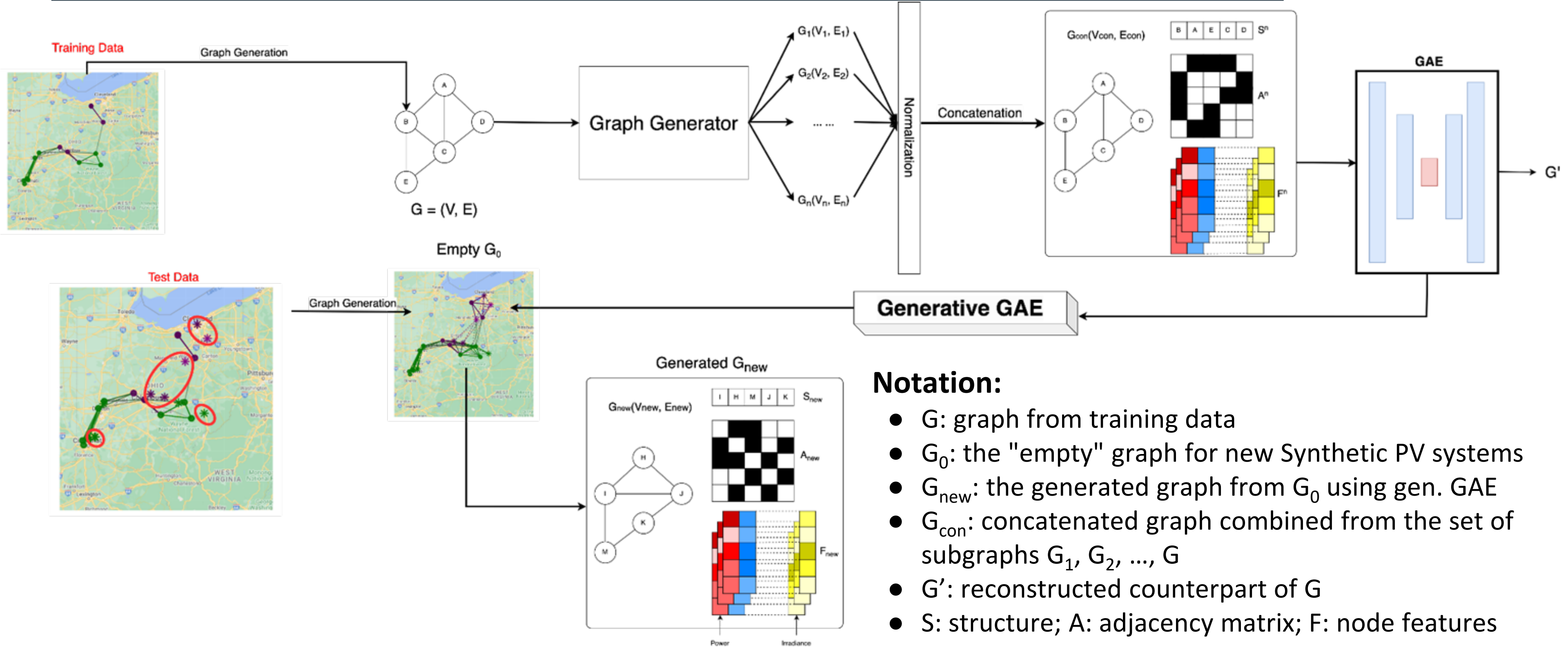
Dynamic st-Graphs for Generating Performance of Virtual PV Systems



Dynamic Graphs

- **Allow for the permutations of the existing graph structure**
  - New Nodes / Edges
  - Directed graphs, to guide imputation of new Virtual PV Systems

Generative AI Modeling



Notation:

- G: graph from training data
- G_0: the "empty" graph for new Synthetic PV systems
- G_{new}: the generated graph from G_0 using gen. GAE
- G_{con}: concatenated graph combined from the set of subgraphs G_1, G_2, …, G
- G’: reconstructed counterpart of G
- S: structure; A: adjacency matrix; F: node features

An Illustration of how to derive the Generative GAE from training data and apply Generative GAE to generate data for new PV systems.

The Challenges, & Opportunities, of AI/ML: Accelerating Time to Science

To develop AI/ML for Science, Such as PV Science

We have High Performance Computing (HPC)

- "Scaled Up" Computing: Works for Physics Simulation Modeling
  - Doesn't handle massive datasets

Yet Big Tech uses Distributed Computing (DC)

- "Scaled Out" Computing: e.g. used by Google, Meta, etc.

AI/ML for Science needs D/HPC Computing

- Needs the integration of "Scaled Out & Scaled Up" Computing
- CRADLEtm: Common Research Analytics & Data Lifecycle Environment[1]
  - Automated pipelines, FAIRification[2], Efficient Insights

Data Centric AI[3] presents humans with a grand opportunity

- "*Computational Inflection Point for Scientific Discovery*"[4]
  - Augmenting human reasoning; Working alongside human researchers
  - Scientific investigations restructured around the "salient human tasks"
    - With computers handling the routine and onerous tasks
    - Supplementing our human capabilities

While decreasing reductionist approaches in scientific research

In SDLE Res. Cntr.

- Dist. Compute
  - 2.5 Pb Cluster
  - 7 TB Ram
  - 1164 CPU Cores
  - 30 GPUs
    - 480 GPU VRAM
    - 384k Cuda Cores
    - 1.2k Tensor Cores
- High Perf. Compute
  - 7152 CPU Cores
- Nvidia AISC 8 DGX
  - 2.5 Tb VRAM
  - 4 Tb RAM
  - 15 Tb nvme storage

1. A. Khalilnejad, ry s;., "Automated Pipeline Framework for Processing of Large-Scale …," PLOS ONE, 15, 12, p. e0240461, Dec. 2020.
2. W. C. Oltjen et al., "FAIRification, Quality Assessment, and Missingness Pattern …, IEEE PVSC, Jun. 2022, pp. 0796–0801.
3. M. H. Jarrahi, et al., "The Principles of Data-Centric AI," Commun. ACM, vol. 66, no. 8, pp. 84–92, Jul. 2023,
4. T. Hope, et al., "A Computational Inflection for Scientific Discovery," Commun. ACM, vol. 66, no. 8, pp. 62–73, Jul. 2023,

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25 UG | 26 GR | 4 Postdocs | 3 Staff | 20 Faculty

1. CRADLE, 2. Data Lifecycle, 3. st-Graphs, 4. Geospatial, 5. XRD, 6. XCT

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