FAIR Computational Workflows



FAIR Data – FAIR workflows provide metadata and provenance to describe the involved data in a systematic, traceable manner.

FAIR Criteria for workflows as digital objects – Workflows encapsulate steps for data cleaning, normalization, and database connectivity.



Carole Goble, Sarah Cohen-Boulakia, Stian Soiland-Reyes, Daniel Garijo, Yolanda Gil, Michael R. Crusoe, Kristian Peters, Daniel Schober; FAIR Computational Workflows. *Data Intelligence* 2020; 2 (1-2): 108–121. doi: https://doi.org/10.1162/dint a 00033

What is a workflow?

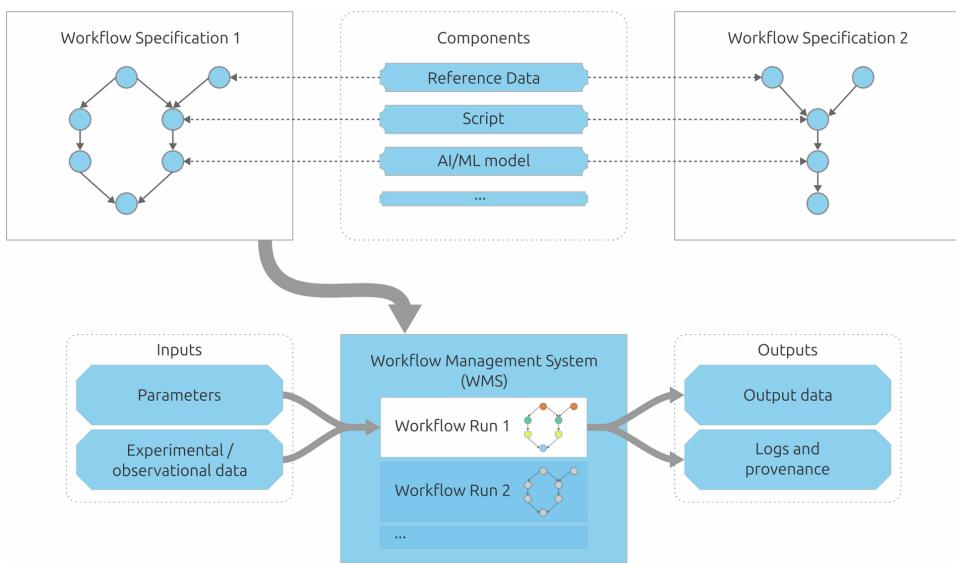


- "Precise description of a procedure"
- Multi-step methods used to curate and steward data.
- Metadata are created throughout measurements, during processing, while tracking data provenance
- "From an execution perspective, workflows are a means to handle the work of accessing an ecosystem of software and platforms, managing data, securing access, and handling heterogeneities."
- For photovoltaics, this involves handling the work of database connectivity, securing access to data, and handling heterogeneities in data.



What is a workflow?





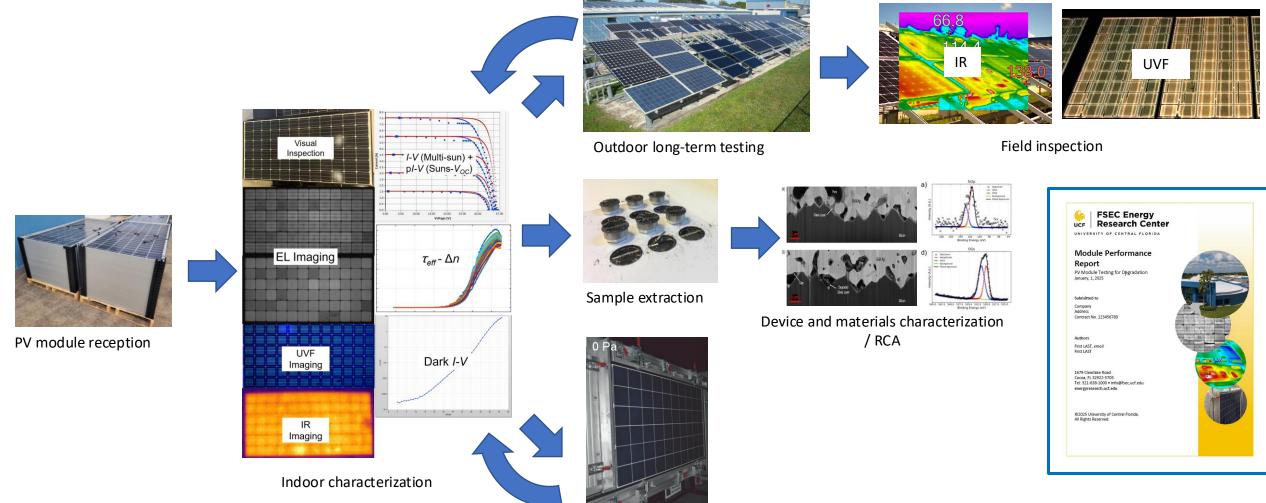


Applied FAIR Computational Workflows in Multimodal Photovoltaic Data Analysis



Life of a Module In Our Facility*





Mechanical loading to simulate extreme weather impacts



*Taken from FSEC Capabilities brochure

PVMCF Data Viewer



Florida-Solar-Energy-Center/PVMCF-Data-Explorer:

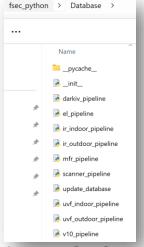
Bespoke data curation tool for the Photovoltaic Module Characterization Facility

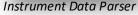
SQLite database automatically generated by metadata parsing scripts.

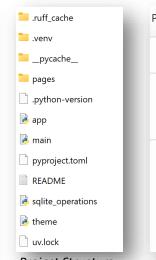
Reactive Shiny frontend allows user to navigate and control program.

Modular and extensible to encourage collaboration and customization.

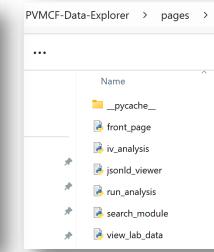
UV package management and dependency environment solving.



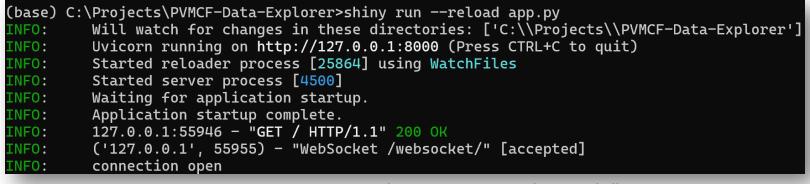




Project Structure

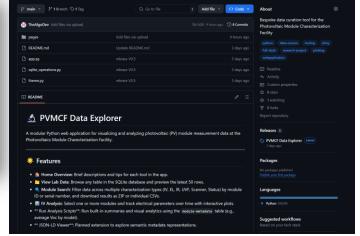


Modular Pages for GUI



Current setup requires running command invocation in anaconda powershell





Hosted on Public GitHub Repo

Home





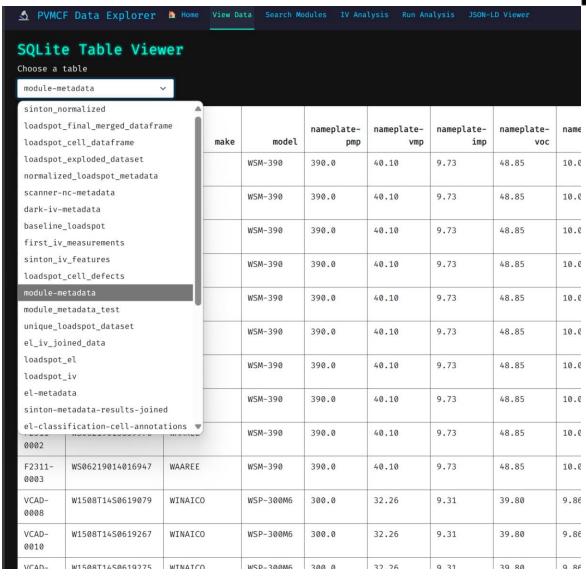
- Home tab provides overview of program capabilities with descriptions of computational workflows.
- Helpful place to start for new users, can include a guide or link tree to relevant materials(SOPs).
- Provides few moments to establish database connections and set up logging.
- Places the user in control of their research experience.



View Data



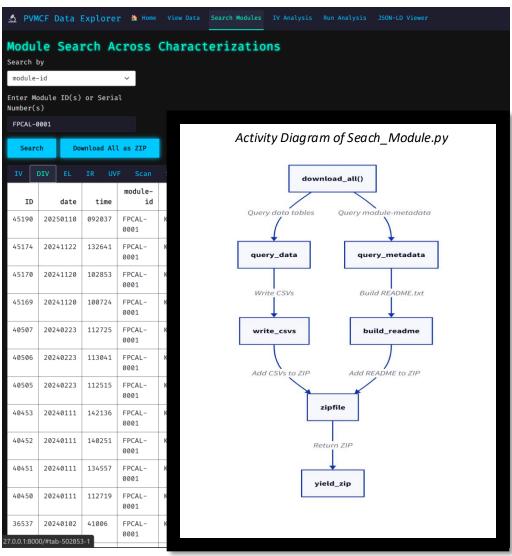
- Data model agnostic module that displays all tables of connected SQLite database.
- DESC SQL keyword implemented to display most recent observations.
- CSVs can be loaded into a SQLite database and viewed here as well.



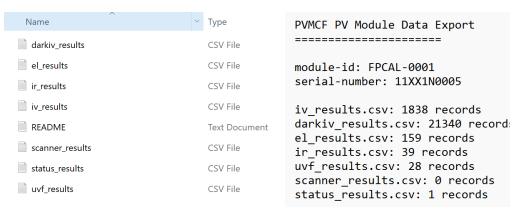


Search Modules





- Early form ideation of Automated Reporting.
- Fully automated data pipeline providing AI ready data for multimodal photovoltaic analysis.
- One click dataset retrieval as compressed zip folder, with customizable metadata reporting.
- Utilizes internal module-id(s) or serial-number(s) to aggregate all data and associated metadata for module(s) processed by the PVMCF.



ZIP output from SQL tables

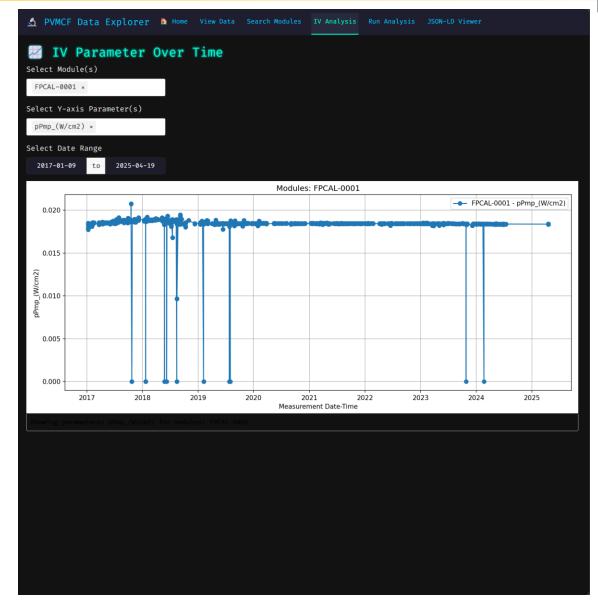
Readme metadata and reporting



IV Analysis

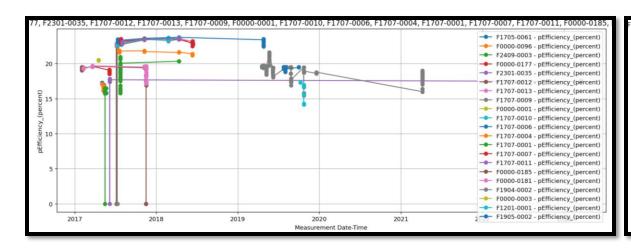


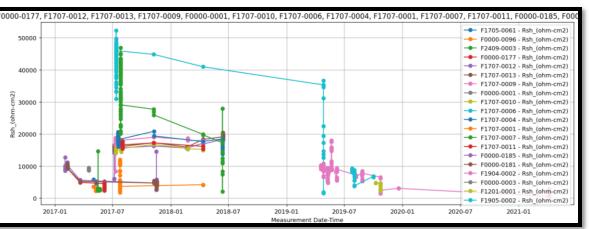
- Dynamic parameter plotting of any variable over the module's history at FSEC.
- Useful for quick checks on a module or set of modules, the plots update in real time.
- Currently limited to SintonFMT-350 with plans to extend using Spire and Time Series Data.
- Next iteration ideas:
 - Multiple Y axis values
 - Export plot to PNG option
 - Export to pickle for aftereffect editing
 - More granularity to adjust plots
 - Display plotted parameter value from both
 Spire and Sinton data on same plot



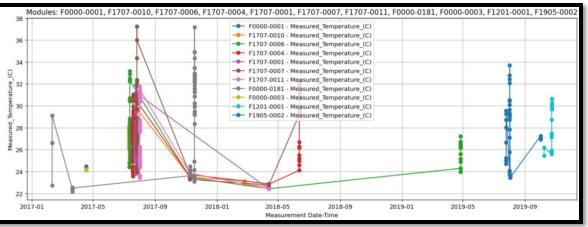
IV Analysis Demo – Subset of Loadspot Modules













Next Steps



- Implement logging
- Integrate Postgres and NSF Access
- Determine what is most useful.
- Create Activity Diagrams for additional workflows and modules.
 - Upload local data to repo
 - Detailed Automated Reporting
 - View raw file from GUI
 - Orchestrate File Transfer
- Further modularize the code to be used by any researcher on their domain.
- Create SOP for adding new modules to program

