Documenting Scientific Workflows: The Metadata, Provenance & Ontology Project

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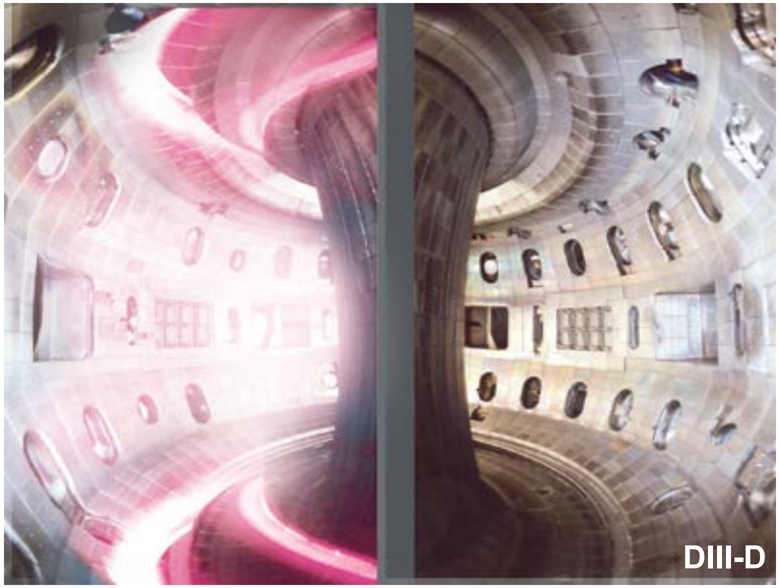
GENERAL ATOMICS

Long History of International Collaboration in Magnetic Fusion Research



- **Data Management for experiments**
  - Client/server worldwide access
  - Metadata for discovery
- **Electronic logbook**
  - ~500,000 entries
  - Real-time and searchable
- **Our science has evolved to rely extensively on modeling**
  - Diverse community extending well beyond the code developers
  - Data management not as comprehensive in the modeling community
- **Desire to create a "scientific notebook" for computational science**
  - Data has enduring meaning; foster collaboration (Greenwald, IAEA, 2011)

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Acknowledging the Support of ASCR & FES as well as the Contributions of the GA, LBNL, and MIT Team Members

- **DOE/SC support critical**
  - Both ASCR and FES
  - Productive partnership going back to the first SciDAC in 2001
  - Fusion Collaboratory, SWIM, Web Portal, Network QoS, ESL, AToM, etc.

- **Thanks LBNL: Arie Shoshoni and Alex Romosan**

- **Thanks MIT/PSFC: Martin Greenwald, Josh Stillerman, John Wright**

- **Thanks GA: Gheni Abla, Bobby Chanthavong/Liz Coviello, Xia Lee**

- **Based on MPO team's 2014 presentations at the APS/DPP Meeting (Greenwald, et al.) and the NGNS PI Meeting (Schissel et al.)**
  - Metadata, Provenance, Ontology (MPO) Project: 9/1/2012 - 8/31/2015

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Objectives: Document Scientific Data Flow

- **Preserve meaning of data by documenting all of the steps taken to produce the data = provenance**
  - Capture both data and process
  - Support more systematic management of analysis & simulation data
- **Provide and preserve answers to two key questions:**
  - Where did a particular piece of data come from?
    - What were the inputs, assumptions and parameters used in its calculation?
    - And where did the inputs come from?
  - Where was this data used?
    - Other calculations
    - Publication or presentation
    - Contributions to databases
- **FES as a test bed but applicable to *all* science domains**

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Example Use Cases

- **How did I arrive at the data plotted in figure 6 of my 2014 Phys. Plasmas article?**
- **A calibration error was found in Thomson Scattering data taken during 2011**
  - the data has now been recalculated, but where was the old data used?
  - What publications used that data? Were they critical for the published conclusions?
  - Did we contribute any of that data to an international database?
- **A recently graduated PhD student left behind output from thousands of gyrokinetic simulations**
  - Which of these were used in her thesis?
  - Which might be useful in the future? What were the inputs and parameters used in the interesting runs?

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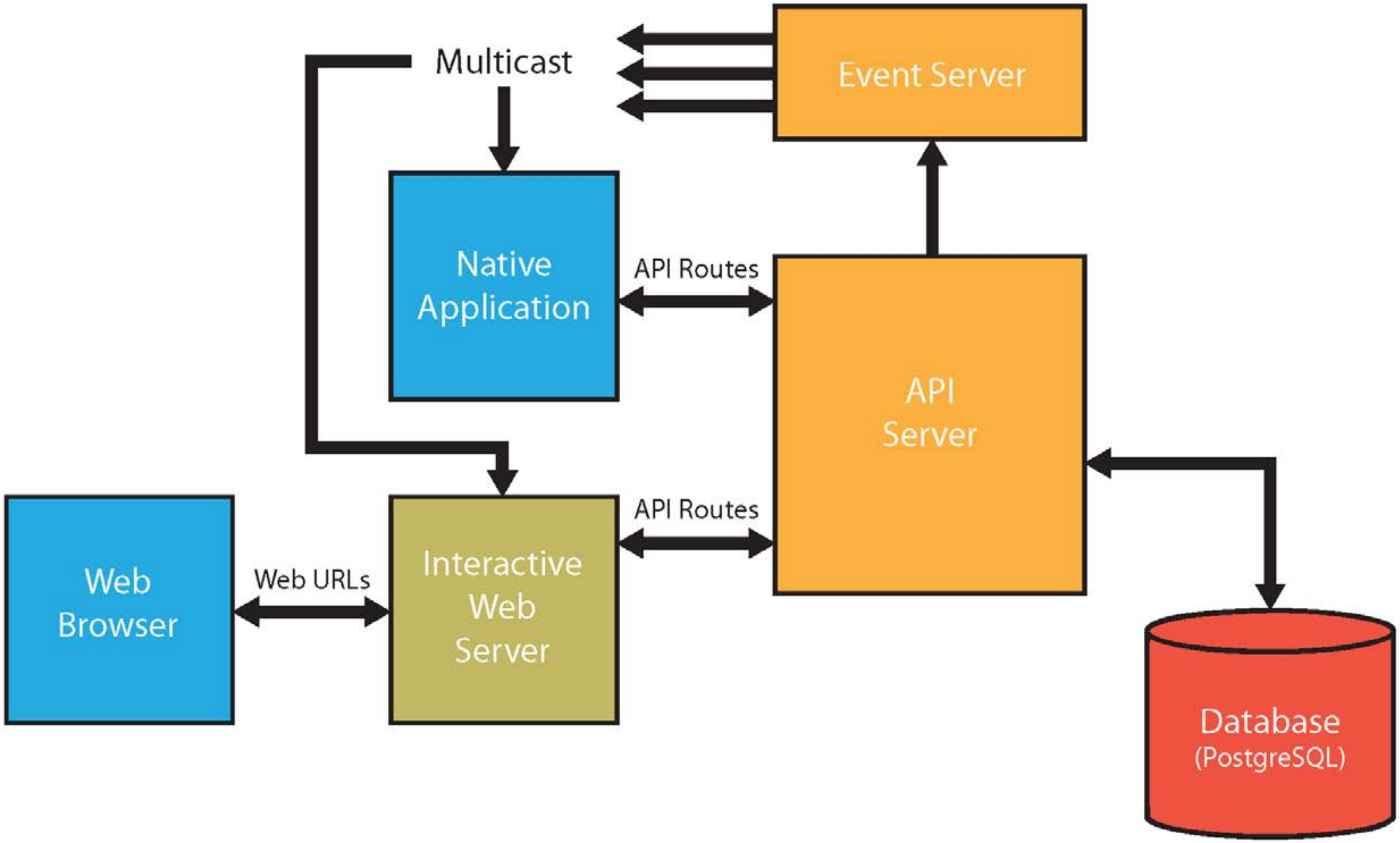
Non-Functional Requirements

- **Support all scientific workflow – experimental & computational**
  - Typically involves processing of raw data, with small or large codes often providing inputs to larger simulations, whose output requires processing as well
- **Allow users to record as much/little information as they need**
- **Function in a heterogeneous environment and interoperate with whatever workflow tools people are already using**
  - Researchers use many different languages (Shell scripts, python, IDL, Matlab, etc.) and tools to get their work done
  - Many different computational platforms – laptop to HPC
  - Data is stored in different formats (MDSplus, HDF5, ASCII, etc.)
  - It would be futile to insist that researchers change all of that to get the benefits that we propose
- **Once set up, needs to work as automatically as possible (so best suited for scripted rather than one-time use)**

Basic Components of the MPO System

- **Database/ Database Server**
  - Captures metadata, location of data, and all processing steps
- **API/ API server (Application Program Interface)**
  - Mediates all communication with database
  - Gives users a language interface to instrument their workflow scripts
- **Web Server**
  - Provides interactive user interface to discover & explore workflows
  - Allows users to enter new comments about any MPO object
- **Event Server**
  - Enables automatic updates of workflow information

Basic Components of the MPO System



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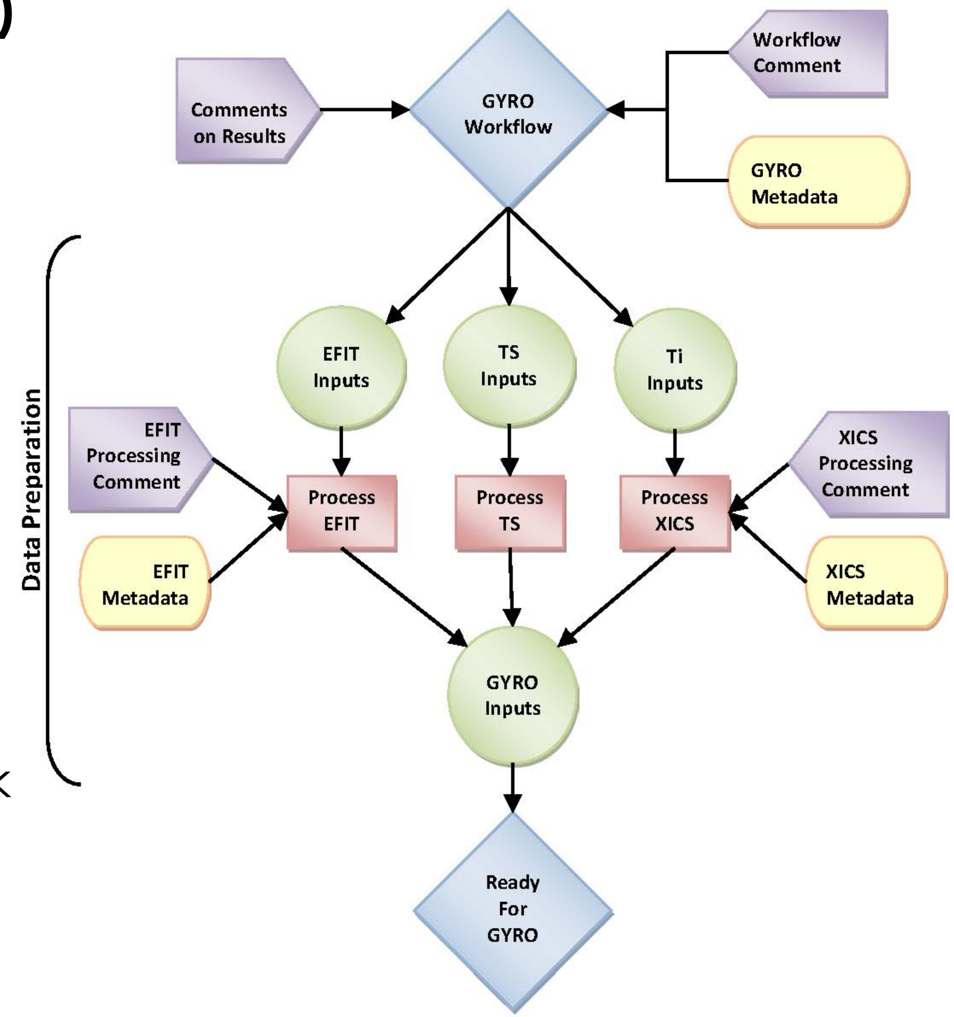
Workflows Depicted as Mathematical Graphs

- **Directed Acyclic Graphs (DAGs)**
  - Directed: flow is defined and one-way
  - Acyclic: Loops are not allowed
  - Graph: Set of objects, connected by links
- **Shows each step in the processing chain**
- **The parent-child relationship is stored and can be followed in either direction**
  - Properties can be inherited
  - Allows simple consistency check e.g. are all parents older than their children?



For Every Record, We Want to Provide Information on "Who, What, When, How, and Why"

- **What: Each object has a user-supplied name and description**
  - Plus contextual information
  - Plus optional metadata
  - Plus data pointers

- **Who and when: Every MPO object is automatically tagged with a time and the user's name**

- **How: Via the workflow connections**

- **Why: Supplied through comments/annotation**

Data Model: What we Store

- **Data objects: Structured data, mostly stored outside the database schema**
  - MPO keeps pointers – in the form of URI (Uniform Resource Identifier) - that uniquely identifies the data and its access method
  - Additional metadata maintained to aid in searching & browsing
- **Activities (actions): Anything that creates, moves or transmutes data from one form to another**
  - Includes data importing, staging, file copying, pre-processing, operation of large and small codes, data writing, post-processing, data exporting
- **Connections: The causal links between inputs, actions & results**
- **Comments: User annotation as unstructured text**
- **Collections: Simple lists of any type of MPO objects, defined by users for any purpose**

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Persistent Data Store: Data Objects Must be Maintained

- **Underlying the model is an assumption that data objects will be maintained**
  - If the underlying data are allowed to change in untracked ways, the descriptions and provenance are corrupted
  - Data can be moved to a new location or converted to a new format – as long as this is written down in the MPO database
- **MPO does not dictate the implementation of the persistent store**
  - Data objects can be a reference to a user's file system
  - Data objects can be a description of how to retrieve the item from a database or record store
  - Data objects can be a description of how to retrieve files or directories from a file store
- **Methods are available to manage persistent store's data in a manner consistent with maintaining the integrity of the MPO system**

Collections

- **Users can define “collections”**
  - Each tagged with description or purpose
- **Arbitrary sets of objects of any kind**
- **Example Uses:**
  - Multiple runs in a parameter scan
  - Workflows that contribute to a particular publication or presentation
- **Objects can be members of any number of collections**
- **Collections of collections can be defined**

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Shared Objects and Connected Workflows

- **Typically a user will employ multiple workflows in a particular application**
  - For example: Code A provides the spatial mapping for raw data; processed data is input into Code B; Code B's output is compared to Code C's output
- **We chose not to define sub-workflows and sub-sub-workflows as too complex and confusing**
- **Instead, workflows are linked via shared data objects**
  - i.e. these data objects have more than one connection
  - Each connection is tagged with the workflow id
  - This provides the head to tail coupling between workflows
  - Shared data objects are highlighted in the user interface, allowing users to navigate from workflow to workflow
  - It allows easy re-use of data objects – a common occurrence

Managing the Namespace

- **Each object in the MPO has a globally unique numerical identifier**
- **Workflows can be found by searching or browsing, but how would you convey that information to someone else?**
  "Take a look at my TRANSP run 1234"
  - We define a composite ID that is easy to remember
- **Each data object is provided with a pointer in the form of a URI**
  - Uniform Resource Identifier,
  - Superset of the URL (Uniform Resource Locator)
  - The URI is the pointer to the data object
- **Searching is enhanced by defining a "controlled vocabulary"**
  - User-defined, hierarchical ontology

Controlled Vocabulary: Ontology

- **In computer science, an ontology is a formal framework for representing information**
- **The MPO employs a user-defined ontology to describe types of metadata**
- **This enhances searching since the vocabulary for a particular application is defined**
  - So in a particular application I can see that I want to search for "confinement_mode" = "H-mode" and not "conf_mode" = "H-Mode" or "Hmode"
- **Users can browse or search the ontology**
- **Users can add terms to the ontology**
- **The MPO ontology is arranged in a hierarchy to enhance browsing**

MPO Project is an *Applied* Computer Science Project

- **MPO software utilizes open source solutions wherever possible**
- **MPO is a "web service"**
- **"PostgresSQL" database used for current implementation**
- **Both API server and Web UI server use "Flask", a lightweight web application framework**
  - API based on REST abstraction = Representational State Transfer
  - Database operations through HTTP verbs (e.g. post) and URLs
- **Twitter "Bootstrap" to create standardized Web front-end**
  - Hides Javascript complexity
- **DAGs rendered by "Graphviz" software**
- **Authentication via x.509 certificates (OSG, MIT & MPO certs)**
- **MDSplus event services**

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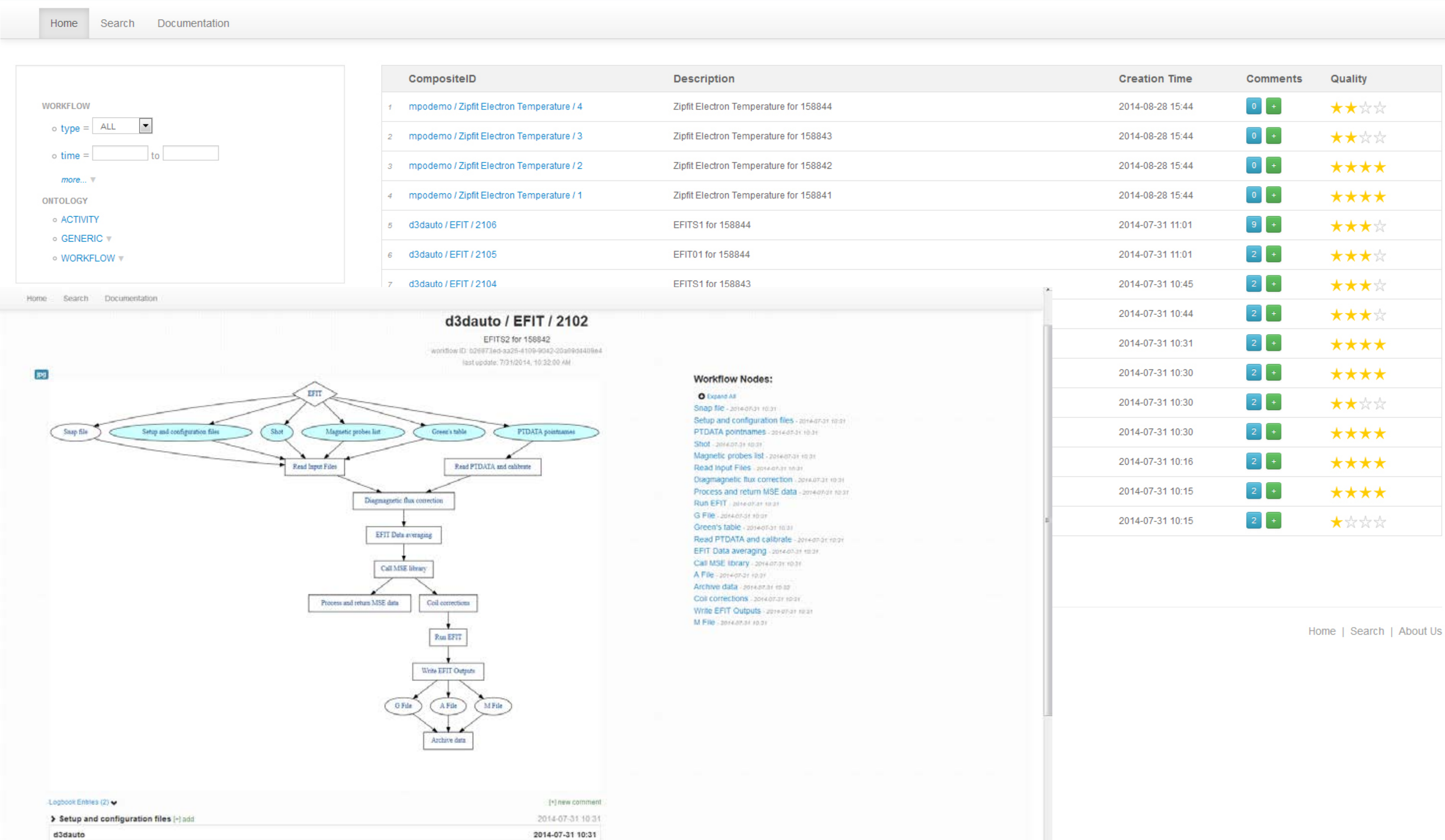
Substantial Progress has been Made

- **Basic components all built**
  - Database schema defined and implemented
  - API available in shell, python, IDL
  - Web-base user interface built - supports searching and browsing, dynamic display of workflows and metadata
- **Production and development environments are available**
- **In the process of beta testing**
  - SWIM, the SWIM Portal, and the AToM Project
  - GYRO
  - EFIT including DIII-D's between shot analysis while operating
  - TORIC
- **Evangelizing the philosophy throughout the community**
  - 3 IAEA/TM papers (2013, 2015), APS/DPP (2014), PI meetings

MPO Web Site Operating with Ontology-based Search, Automatic Real-Time Graphics, Live Data Loading



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Project's Final Year Goal is to Expand System's Depth and Expand the Reach of our Tools into other Sciences

- **Taking on friendly beta users**
  - Presentation at APS/DPP Nov. 2014 (attracted beta users)
  - Support other languages, add requested features, documentation

- **Beginning to work with a difference science domain**
  - CASCADE Project: DOE's Regional/Global Climate Modeling Program

- **Hardening for Production**
  - Formalize schema updates, separate development/production/user sandbox, develop/guarantee our persistent store

- **Continue to evolve MPO UI and data schema**
  - For example: UI evolving to handle large quantity of workflows, adding collections

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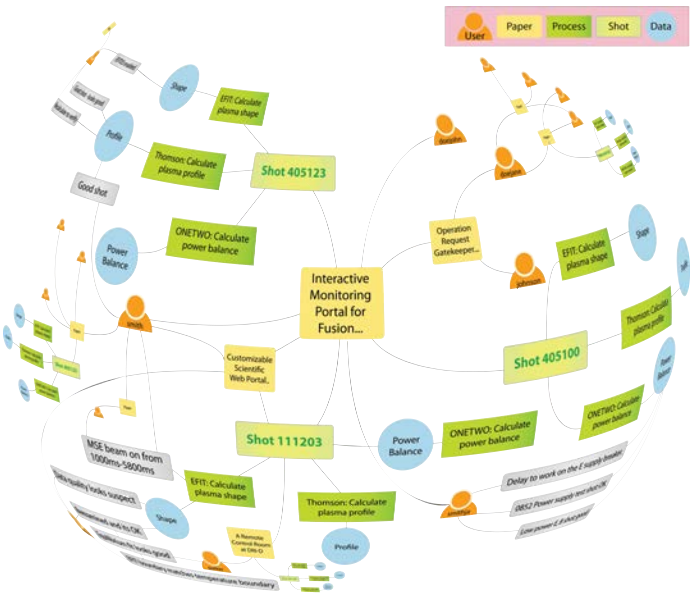
Questions We are Asking Ourselves Today

- **How to expand the reach of our MPO framework?**
  - Across many science domains (ease of adoption, robust)
  - Federated system within a science (fast at large scales)
- **Compatibility with W3C Standards (e.g. PROV)**
  - How to import/export to MPO?
  - Can draw in this ecosystem (e.g. Annotation WG)?
- **Efficient UI operation at large-scale**
  - How to do better/faster Graphical Navigation?
- **Provide rich data centric tools**
  - Are there different UIs to the MPO data?



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Summary

- **Substantial progress towards a production system**
  - API, data store/Ontology, & UI all evolved
- **Production workflows have been MPO instrumented**
  - DIII-D experimental analysis & SWIM simulations
- **Our results validate our approach**
  - Simple API to instrument basically any existing workflows
  - General data store and UI to store and navigate
- **Include Climate Modeling science domain moving forward**
  - Yield feedback to allow iteration on the MPO framework
- **Presentation at the 10th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation in Fusion Research**