Automated Metadata, Provenance Cataloging and Navigable Interfaces: Ensuring the Usefulness of Extreme-Scale Data*

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Insuring the Usefulness of Extreme-Scale Data: System for Fusion Science Operational

Objectives:

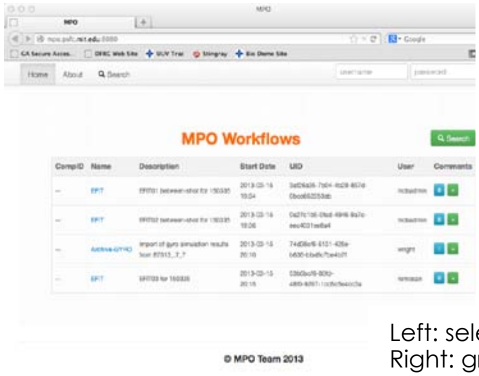
- Create a data model, infrastructure, and a set of tools to automatically document workflow & data provenance from any tool that processes data
- For each data element: who, what, when, how, why including tracking connections & dependencies between data elements
- Deploy interactive tools for efficient browsing and searching of workflows & associated data
- Production deployment on real-world fusion data
- Extend solution to other sciences within SC portfolio

Approach:

- Integrated metadata, provenance & ontology system
- Primitive and languages for annotation
- Database schema design for general solution
- Research on user interfaces: graphical navigation
- Demonstrate on real-world fusion applications with early deployment & agile development
- Extend to other sciences to validate generality

Progress:

- Data being loaded, system being refined based on feedback



MPO Workflows

CompID	Name	Description	Start Date	UID	User	Comments
--	EFIT	EFIT01 between-shot for 150335	2013-03-15 19:04	3a026a36-7b04-4b28-857d-0bcd6825 53db	mcbadmin	
--	EFIT	EFIT02 between-shot for 150335	2013-03-15 19:06	0a27c1b5-0fad-4846-9a7c-eec4031ee8a4	mcbadmin	
--	Archive-GYRO	Import of gyro simulation results from 87313_7_7	2013-03-15 20:10	74d08ef6-6131-426e-b630-bbd[illegible]	wright	
--	EFIT	EFIT03 for 150335	2013-03-15 20:15	036b0[illegible]	[illegible]	

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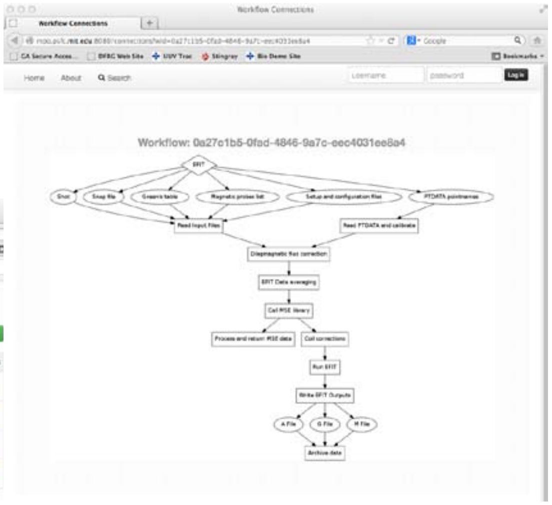


Left: selection screen for previously run workflows.
Right: graphical presentation of a selected workflow.

Impact:

- Increase the value of experimental & computational data across the diverse domains of the DOE/SC
- Paper presented in China at an IAEA meeting solicited substantial interest from attending scientists
- Operational system deployed for alpha/beta users that supports data provenance, metadata, and ontology with interactive tools for browsing and searching

3-year project started October 2012
Contact: D. Schissel (schissel@fusion.gat.com)

Tracking of the Data Lineage has not kept Pace with the Explosive Growth in the Amount of Data

- **Provenance: from the French *provenir* “to come from”**
  - Where did a piece of data come from & where was it used
- **Questions that data provenance can answer**
  - *Diagnostic X* calibration changed, what about my results?
  - What data/publications does this code bug effect?
- **Associated questions that can be answered**
  - Who does “*Analysis Y*” so I can ask for advice?
  - Who else is analyzing this shot in detail?
- **DOE Digital Data Management Statement (July 2014)**
  - All stages of the digital data lifecycle: Capture, analysis, sharing, and preservation
  - Data Management Plans now required

Goal: Support Data Tracking, Cataloging and Integration Across a Large Scientific Domain

- **Create a data model, infrastructure, and set of tools**
  - Automatically document workflow and data provenance from user scripts or any tools that process data

- **For each data element: who, what, when, how, why**
  - Connections & dependencies between data elements
  - Human or automated annotation

- **Realistic applications starting with Fusion research**
  - What scientists do today (e.g. shell, Python, IDL, MATLAB)
  - Vision: an API that can be applied to any tools used to process or manipulate data (experiments & HPC)
  - Not tied to a specific workflow engine

Approach: Focused Research to Build Tools for Real-World Science

- **Integrated metadata, provenance & ontology research**
  - General data model and conceptual framework
  - Directed Acyclic Graph: Logic of tasks performed
- **Research on User Interfaces: Graphical Navigation**
  - Efficiently browse and search for discovery of workflows, their components, and associated metadata
- **Demonstrate on real-world fusion applications**
  - Early deployment & agile development approach
  - Feedback and improve the design
- **Extend to other sciences to validate our generality**
  - Climate modeling and space sciences

The MPO System has 5 Basic Elements

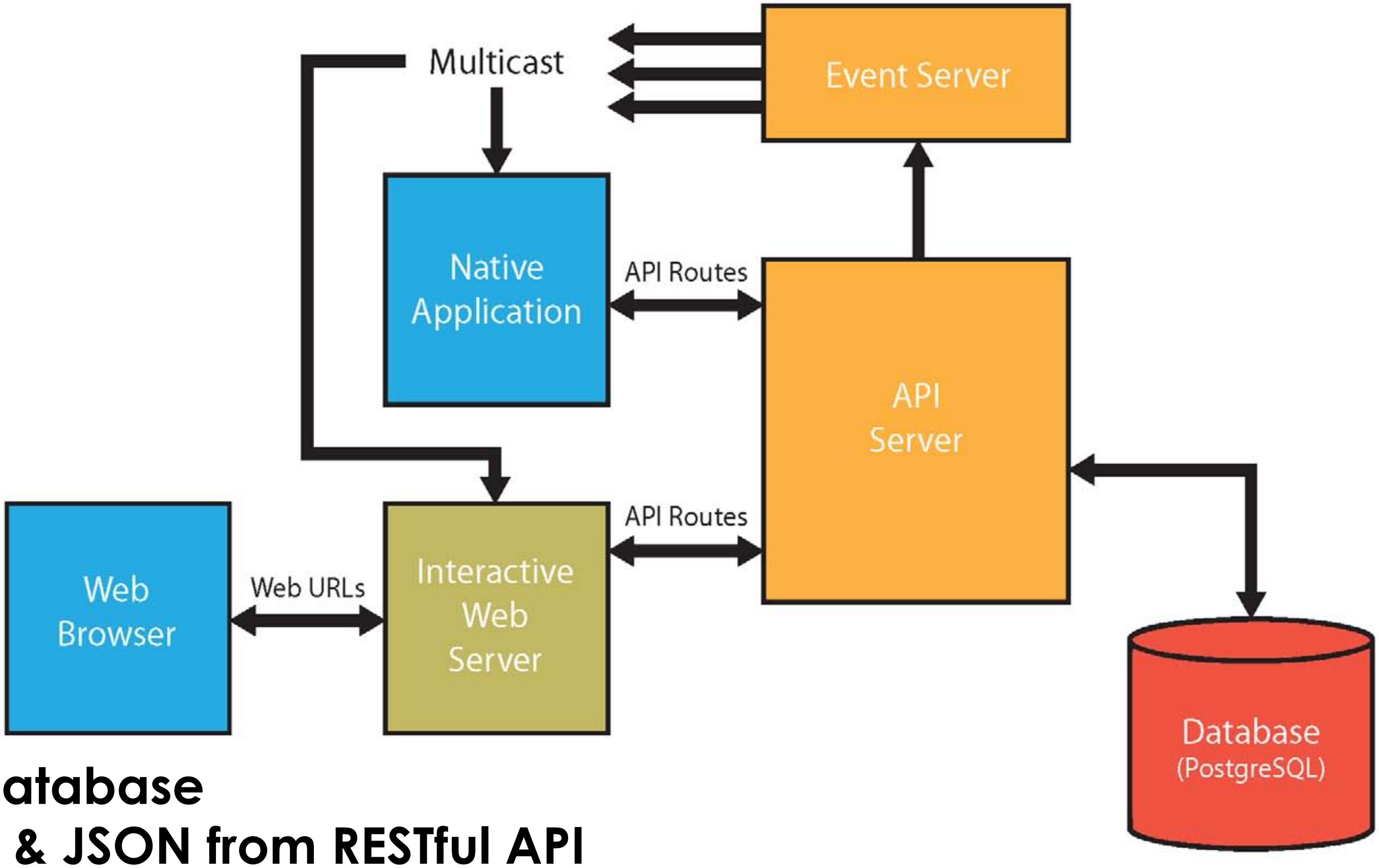
- **Data Objects**
  - Structured data inside/outside the MPO with pointers
- **Activities**
  - Create, move, or transmute data from one form to another
- **Connections**
  - Data objects & activities linked to represent a workflow
- **Comments**
  - Unstructured text with other attributes (e.g. who)
- **Collections**
  - List of related objects, activities, or workflows

Project Divided into 4 Distinct Elements

- **API: primitives and languages for annotation**
  - Useful/realistic for workflow steps data & metadata entry
- **Database: metadata, provenance, ontology, workflow documentation**
  - Capture all elements needed when a workflow executes
- **UI: graphical navigation including real-time updates**
  - Display, navigate, interact, browse the metadata catalog
  - Graphical display to explore workflow and provenance
- **Users: Continual deployment/testing**
  - Starting with EFIT, SWIM, and GYRO from fusion science

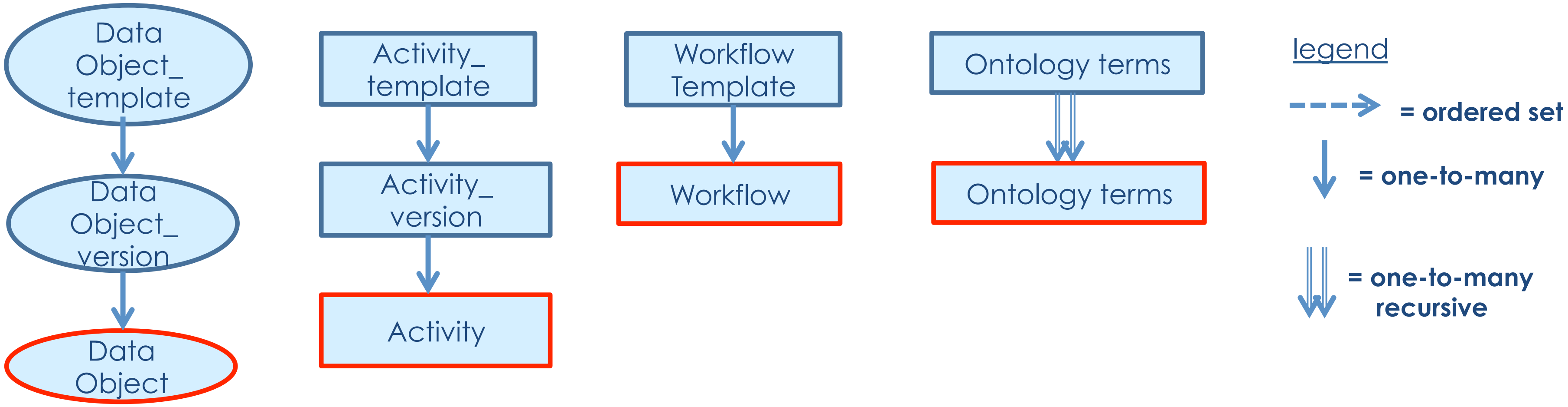
Functional MPO Infrastructure is based on Model-View-Controller (MVC) Concept

- Separates data representation & user's interaction with it



Model = Database
Views = UI & JSON from RESTful API
Controller = Logic on client response or DB interaction

Present Schema Implementation



Data Object_ template

Data Object_ version

Data Object

Activity_ template

Activity_ version

Activity

Workflow Template

Workflow

Ontology terms

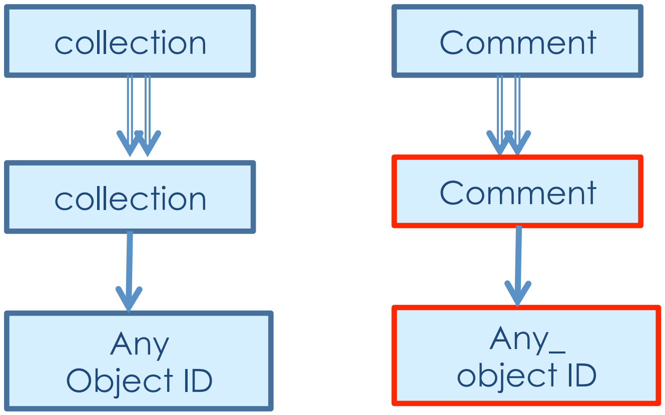
Ontology terms

legend

= ordered set

= one-to-many

= one-to-many recursive



collection

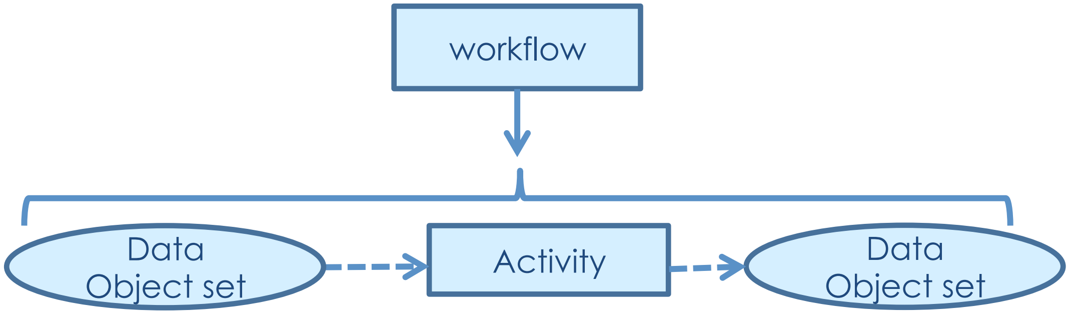
collection

Any Object ID

Comment

Comment

Any_ object ID



workflow

Data Object set

Activity

Data Object set

Connectivity

UI Vision: Integrated Interface for Accessing all Types of Data in a Scientific Environment

- **One intuitive interface to accelerate scientific discovery**
  - Data, data analysis methods, interactive vis, collaboration
  - Hypertext based and graphical

- **Context enable navigation**
  - Search, navigate, interactive access to MPO data
  - Search & navigation directed by domain specific ontology

- **Graphical navigation**
  - Flow chart, flow map, Timeline, Radial Tree map, news-map, tag-cloud maps

- **Dynamic visualizations created from MPO data**
  - Real-time feedback

MPO Software Stack Combines Open Source Solutions

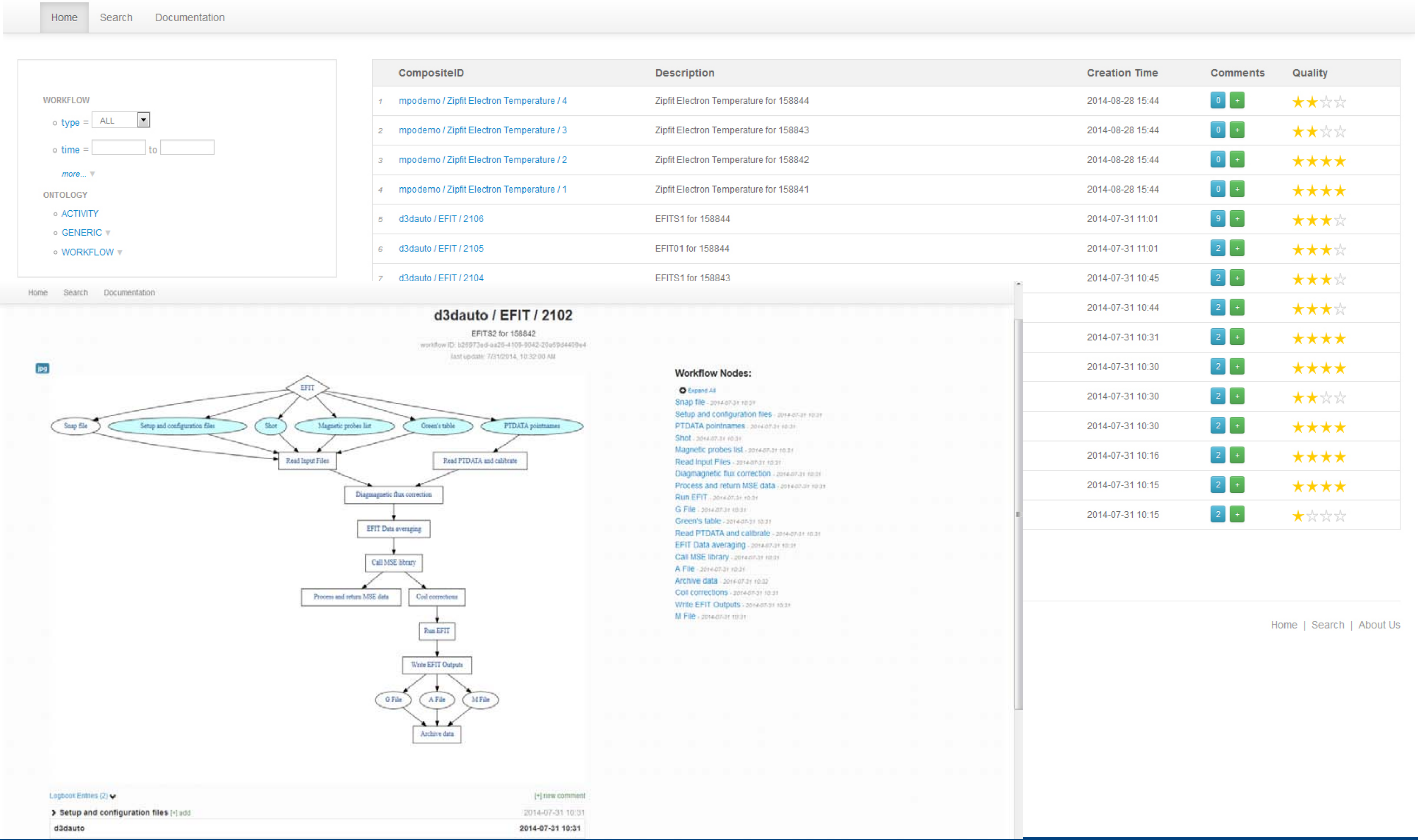
- **Both API server and Web UI server uses Flask - a lightweight web application framework**
  - Core components simple but extensible
  - Supports templates or HTML placeholders
  - Clean separation of components

- **Twitter bootstrap to create standardized Web front-end**
  - Hides Javascript complexity for easier development
  - Built-in responsive web page creation capability

- **DAGs created by Graphviz software package**
  - Dynamically created and embedded in HTML webpage

- **MDSplus event services to create simple event server**
  - Provides real-time update capabilities

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



WORKFLOW
- type = ALL
- time = to

more...

ONTOLOGY
- ACTIVITY
- GENERIC
- WORKFLOW

	CompositeID	Description	Creation Time	Comments	Quality
1	mpodemo / Zipfit Electron Temperature / 4	Zipfit Electron Temperature for 158844	2014-08-28 15:44	0 +	★★☆☆
2	mpodemo / Zipfit Electron Temperature / 3	Zipfit Electron Temperature for 158843	2014-08-28 15:44	0 +	★★☆☆
3	mpodemo / Zipfit Electron Temperature / 2	Zipfit Electron Temperature for 158842	2014-08-28 15:44	0 +	★★★★
4	mpodemo / Zipfit Electron Temperature / 1	Zipfit Electron Temperature for 158841	2014-08-28 15:44	0 +	★★★★
5	d3dauto / EFIT / 2106	EFITS1 for 158844	2014-07-31 11:01	9 +	★★★☆
6	d3dauto / EFIT / 2105	EFIT01 for 158844	2014-07-31 11:01	2 +	★★★☆
7	d3dauto / EFIT / 2104	EFITS1 for 158843	2014-07-31 10:45	2 +	★★★☆
			2014-07-31 10:44	2 +	★★★☆
			2014-07-31 10:31	2 +	★★★★
			2014-07-31 10:30	2 +	★★★★
			2014-07-31 10:30	2 +	★★☆☆
			2014-07-31 10:30	2 +	★★★★
			2014-07-31 10:16	2 +	★★★★
			2014-07-31 10:15	2 +	★★★★
			2014-07-31 10:15	2 +	★☆☆☆

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d3dauto / EFIT / 2102

EFITS2 for 158842

workflow ID: b26973ed-aa26-4109-9042-20a69d4409e4

last update: 7/31/2014, 10:32:00 AM

Workflow Nodes:

● Expand All

Snap file - 2014-07-31 10:31
Setup and configuration files - 2014-07-31 10:31
PTDATA pointnames - 2014-07-31 10:31
Shot - 2014-07-31 10:31
Magnetic probes list - 2014-07-31 10:31
Read Input Files - 2014-07-31 10:31
Diagmagnetic flux correction - 2014-07-31 10:31
Process and return MSE data - 2014-07-31 10:31
Run EFIT - 2014-07-31 10:31
G File - 2014-07-31 10:31
Green's table - 2014-07-31 10:31
Read PTDATA and calibrate - 2014-07-31 10:31
EFIT Data averaging - 2014-07-31 10:31
Call MSE library - 2014-07-31 10:31
A File - 2014-07-31 10:31
Archive data - 2014-07-31 10:32
Coil corrections - 2014-07-31 10:31
Write EFIT Outputs - 2014-07-31 10:31
M File - 2014-07-31 10:31

Logbook Entries (2) [+] new comment

› Setup and configuration files [+] add 2014-07-31 10:31

d3dauto 2014-07-31 10:31

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

- **Alpha Users evaluating, beta users by end of CY14**
  - Presentation at APS/DPP Nov. 2014 (attracting beta users)

- **1st Quarter CY15, push to a different science domain**
  - Which domain depends on who can give us the time

- **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

Summary

- **Substantial progress since the last PI meeting**
  - API, data store/Ontology, & UI all evolved

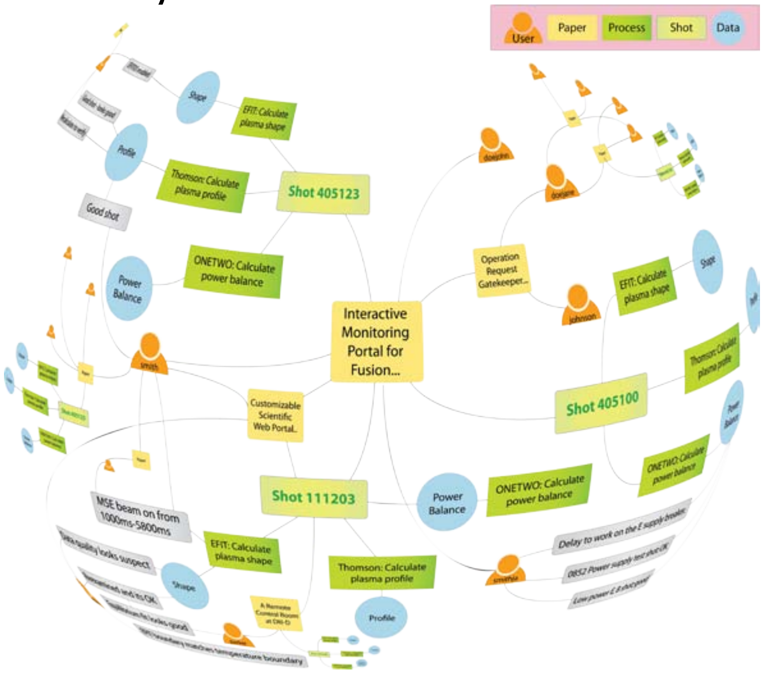
- **Production workflows have been MPO instrumented**
  - DIII-D experimental analysis & SWIM simulations

- **Our results validate our approach**
  - Simple API to instrument basically any existing workflows
  - General data store and UI to store and navigate

- **Include a new science domain moving forward**
  - Yield feedback to allow iteration on the MPO framework

From Rich: “What Question Does Your Research Motivate You To Now Ask?”

- **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?


User
Paper
Process
Shot
Data
Shape
EFIT: Calculate plasma shape
Profile
Thomson: Calculate plasma profile
Shot 405123
Good shot
Power Balance
ONETWO: Calculate power balance
smith
Interactive Monitoring Portal for Fusion...
Customizable Scientific Web Portal...
Shot 111203
MSE beam on from 1000ms-5800ms
EFIT: Calculate plasma shape
Shape
A Remote Control Room at DIII-D
Thomson: Calculate plasma profile
Profile
doejohn
doejane
Operation Request Gatekeeper...
johnson
EFIT: Calculate plasma shape
Shape
Thomson: Calculate plasma profile
Shot 405100
Power Balance
ONETWO: Calculate power balance
Power Balance
ONETWO: Calculate power balance
smithjo
Delay to work on the E supply breaker
0852 Power supply test shot OK
Low power E shot good