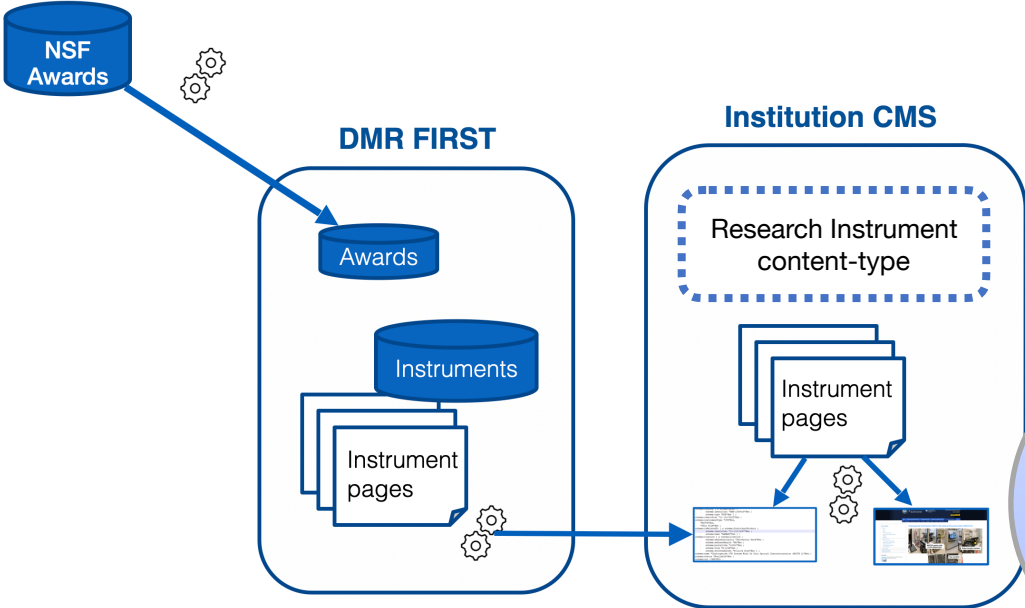


# DMR FIRST Update



Kevin Dressler



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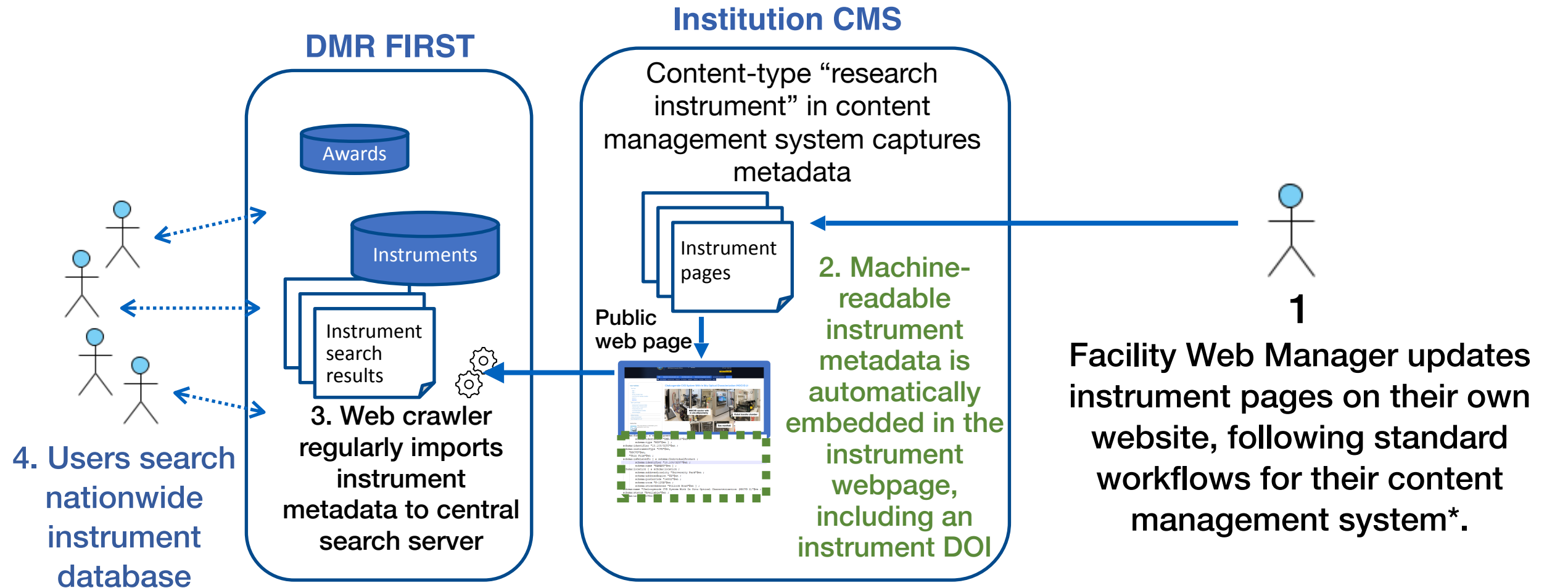


Harshit Jain

MRSEC Directors Meeting, February 2024

# Facilities and Instrumentation Research Search Tool

A federated database of materials instrumentation (DMR-supported and beyond) that updates automatically as facility web managers update their own websites, with a central server that enables global search of rich instrument metadata.



\*or on the DMR-FIRST server, in hosted mode.

# A federated database of DMR-supported instruments

- Instrument data is entered & updated by PIs and their delegates in their own facility websites following current workflows. **If an instrument lacks a website or does not use a content management system, the DMR-FIRST server can provide one that can be inserted into the institutional web presence through “hosted mode”.**
- The facility’s content management system automatically embeds machine-readable instrument metadata into the instrument webpage, using a “research-instrument” content type provided by DMR-FIRST (or home-grown content-types that use our schema).
- The DMR-FIRST server crawls these pages (similar to how a search engine gathers information) to populate and update the central database.
- Instruments can be searched by location, capability, access, per-publication, etc.
- Instrument DOIs are automatically assigned and can be used in publications, etc. to document instrument use and impact.

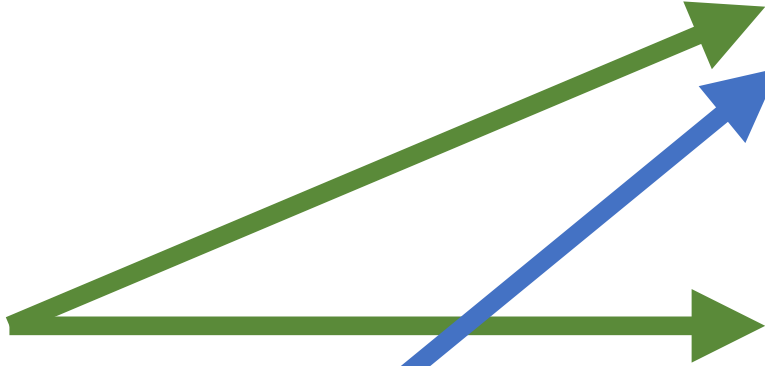
# Use cases

**Instrument Users**



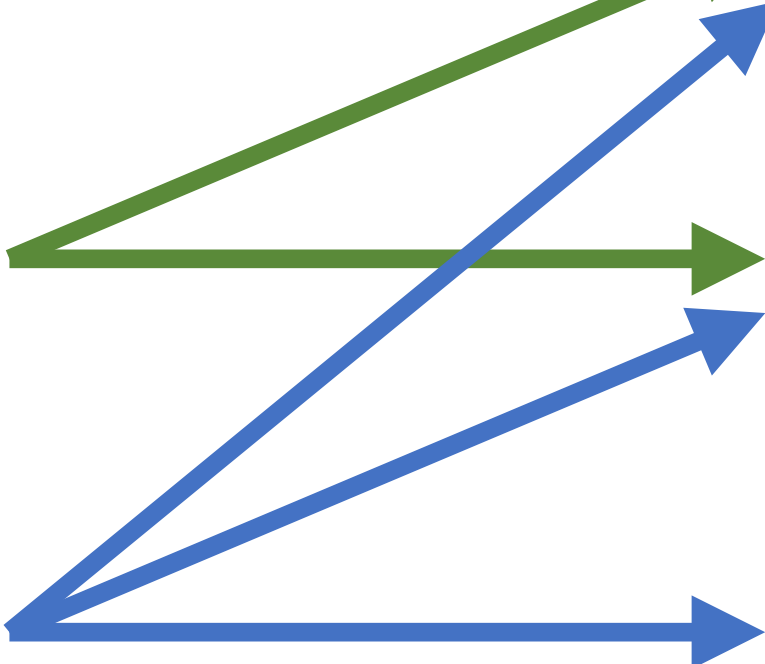
**Search Instruments**

**Agencies**



**Track Instrument Impact**

**Instrument Hosts**



**Update Instrument Information**

# Instrument Hosts

What grants benefitted from this instrument, into which we contributed institutional resources?

What is the impact of our instruments? What publications made use of them?



**University Administration**

- Instrument DOIs track publication impact and which grants benefit from which instruments.

# Instrument Hosts

I only want to deal with updating the instrument information on our own website....

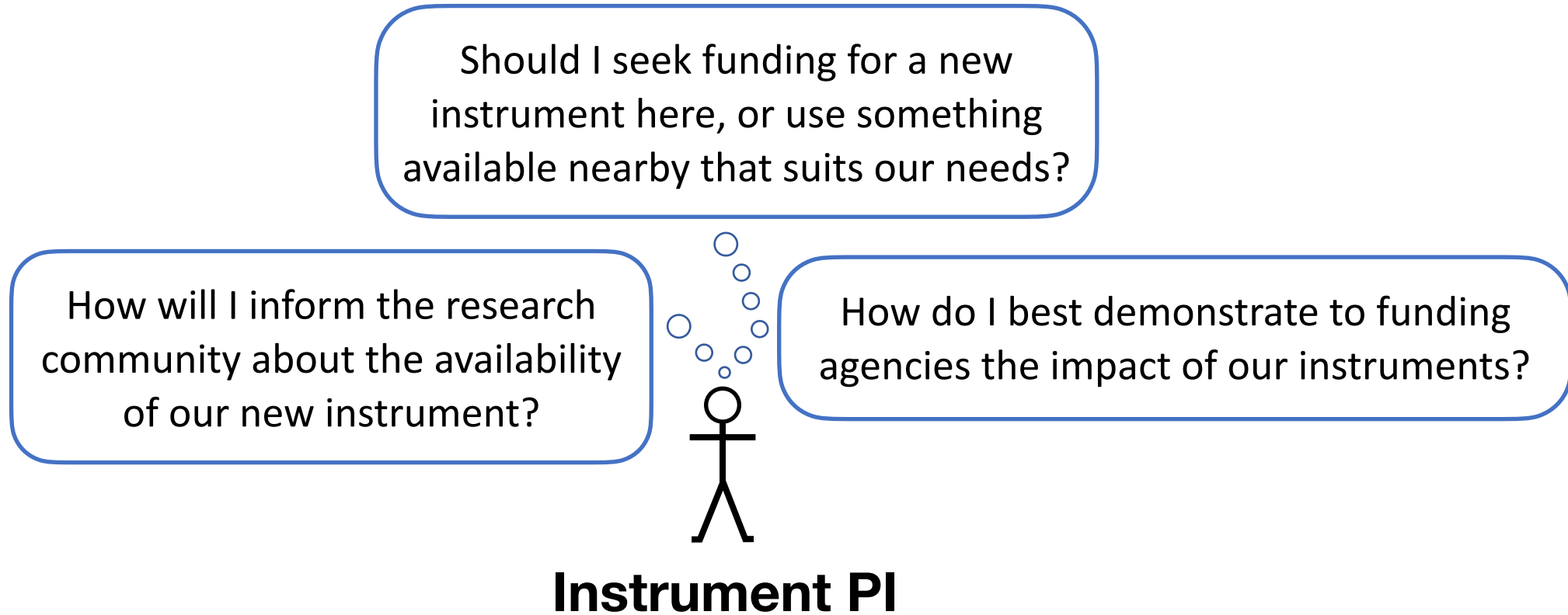
...but getting more external users and tracking the research productivity of our instruments would be great.



## **Facility Manager, DMR Center/Platform Director**

- Manage instrument data within existing content management systems with a DMR-FIRST plugin that can be styled by web managers.
- Instrument DOIs in publications document instrument impact.

# Instrument Hosts



- Pre-award, instrument discovery informs whether to seek new instrument funding and helps make the case that one can secure a broad base of instrument users.
- Post-award, DMR-FIRST can provide a webpage (in the institutional context) as the instrument's public face without additional burden on local web managers.

# Instrument Users

What instruments are available for my research, and how can I access them?

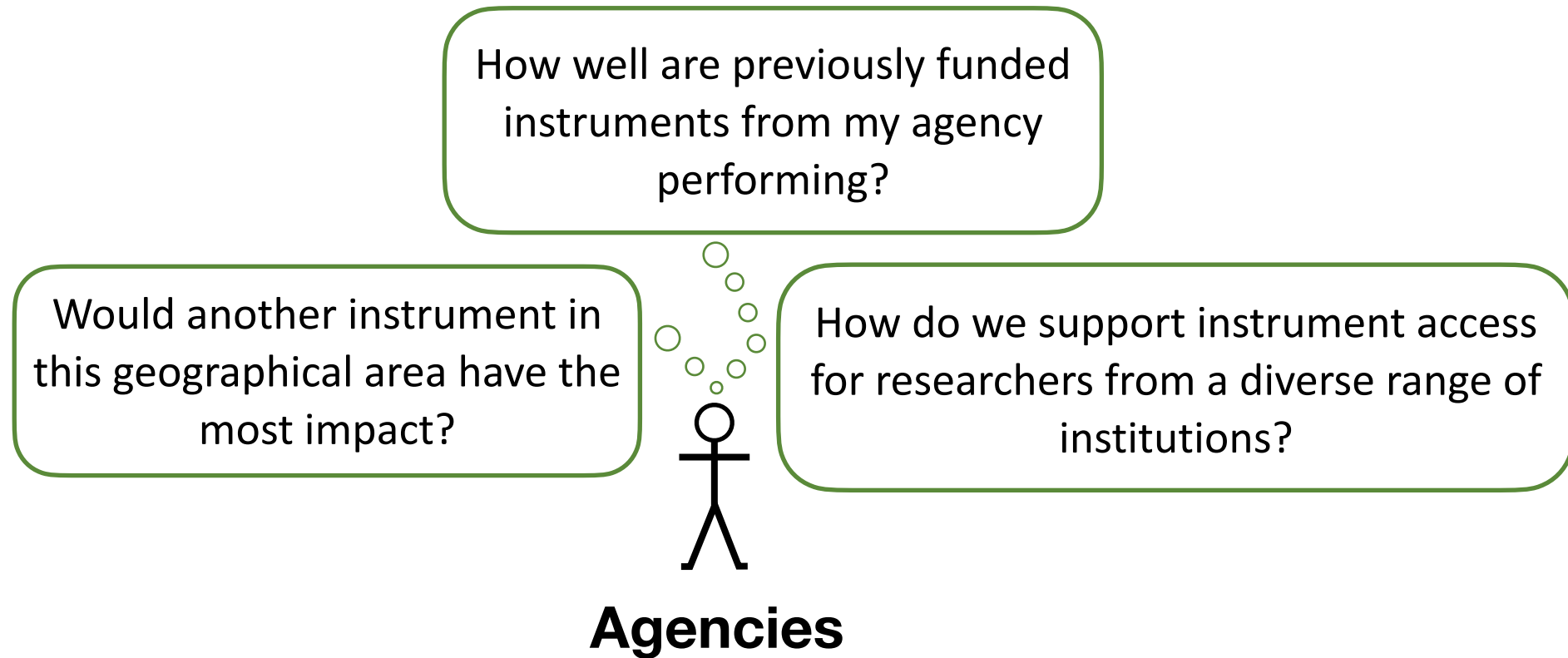


## Instrument Users

- DMR FIRST helps find instruments nearby (or with remote access).
- Standardized, up-to-date information facilitates instrument comparisons, while publications linked to instruments provide examples of instrument capabilities.
- Data scientists can use instrument DOIs for data analytics.



# Agencies

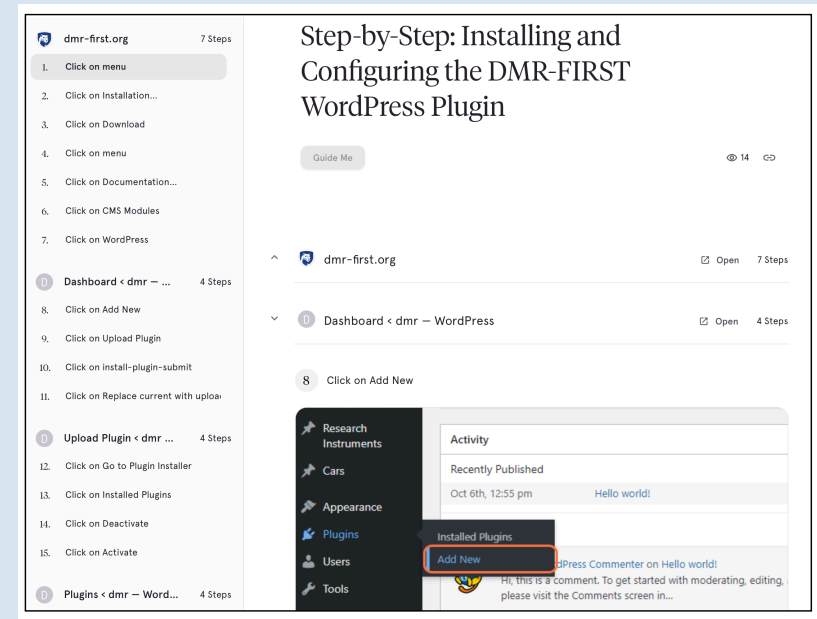


- DMR FIRST can increase awareness and access to instruments, and enable analytics of instrument interest, distribution, use, and impact.

# Updates

## Launched password-accessible [dmr-first.org](https://dmr-first.org)

- **Support pages for plugin download and installation, FAQ, installation walk-throughs.**
- Plugin repository with automated creation of installable plugin versions



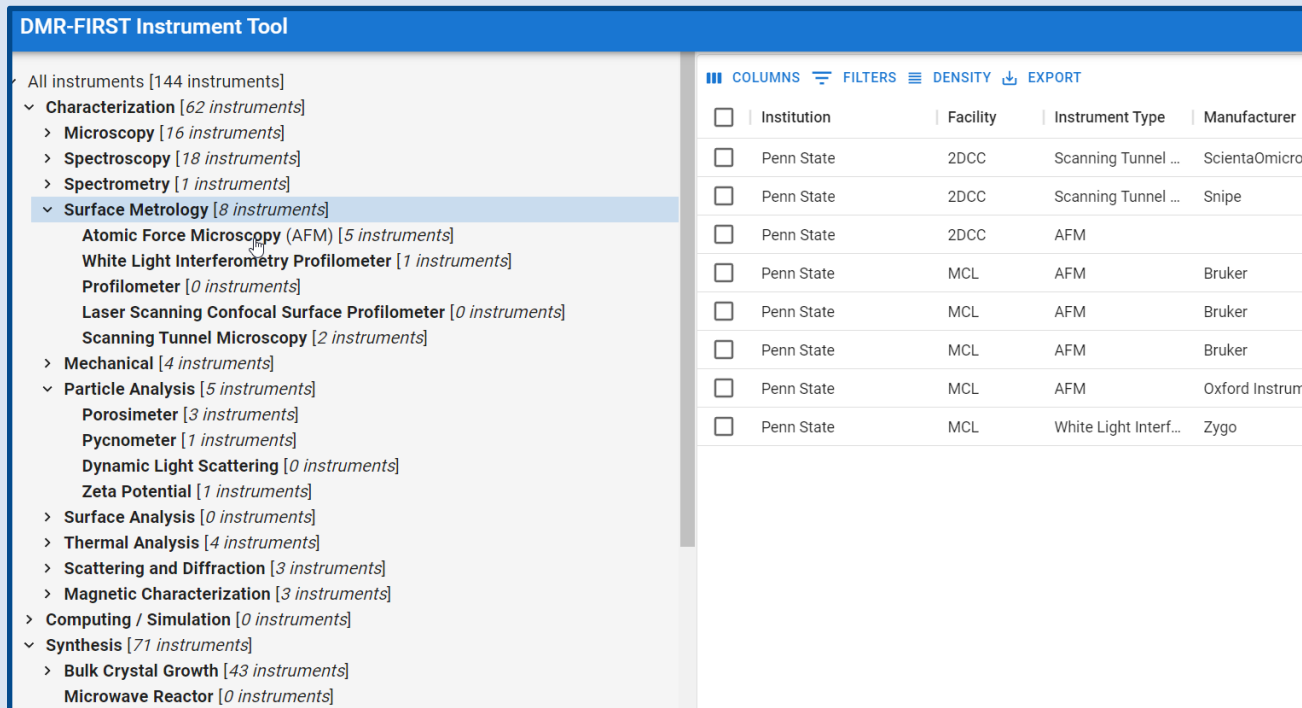
## Updated Drupal module to support versions 9 & 10

- Earlier versions reaching end-of-life.
- **Better support for those who use their own instrument content-type.**  
(Generator of machine-readable data separated from the content-type definition).

## Updated the web crawler

- Discovers all instruments within a given facility website and handles updated and missing/decommissioned instruments.

Implemented **linked instruments** (i.e. cluster tools), **instrument version control** for major (new-DOI) and minor updates of functionality, and an administrative interface on the DMR-FIRST server for database management.



The screenshot shows the 'DMR-FIRST Instrument Tool' interface. On the left is a tree view of instrument types, and on the right is a table of instrument data.

**DMR-FIRST Instrument Tool**

**Left Panel (Instrument Ontology):**

- All instruments [144 instruments]
- Characterization [62 instruments]
  - Microscopy [16 instruments]
  - Spectroscopy [18 instruments]
  - Spectrometry [1 instruments]
  - Surface Metrology [8 instruments] (highlighted)
    - Atomic Force Microscopy (AFM) [5 instruments]
    - White Light Interferometry Profilometer [1 instruments]
    - Profilometer [0 instruments]
    - Laser Scanning Confocal Surface Profilometer [0 instruments]
    - Scanning Tunnel Microscopy [2 instruments]
  - Mechanical [4 instruments]
- Particle Analysis [5 instruments]
  - Porosimeter [3 instruments]
  - Pycnometer [1 instruments]
  - Dynamic Light Scattering [0 instruments]
  - Zeta Potential [1 instruments]
- Surface Analysis [0 instruments]
- Thermal Analysis [4 instruments]
- Scattering and Diffraction [3 instruments]
- Magnetic Characterization [3 instruments]
- Computing / Simulation [0 instruments]
- Synthesis [71 instruments]
  - Bulk Crystal Growth [43 instruments]
  - Microwave Reactor [0 instruments]

**Right Panel (Table):**

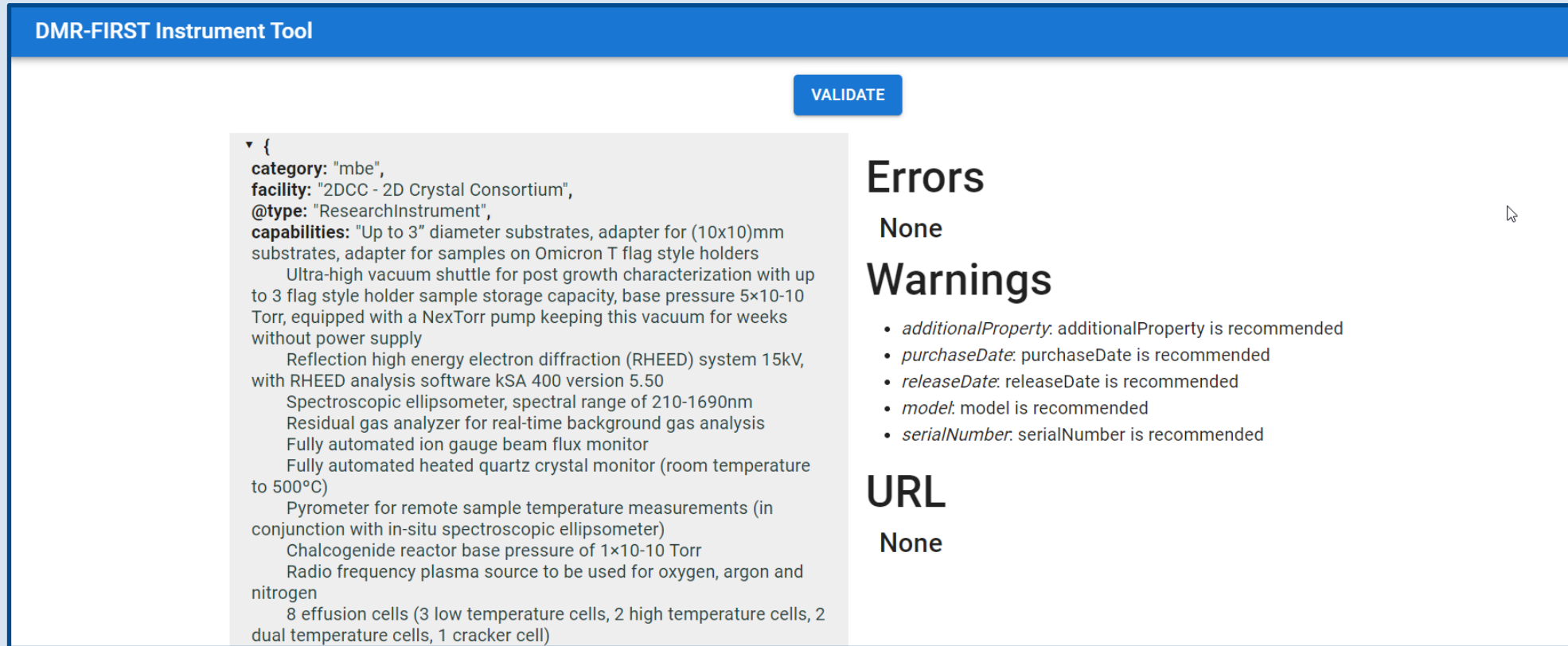
Columns: Institution, Facility, Instrument Type, Manufacturer

Institution	Facility	Instrument Type	Manufacturer
Penn State	2DCC	Scanning Tunnel ...	ScientaOmicron
Penn State	2DCC	Scanning Tunnel ...	Snipe
Penn State	2DCC	AFM	
Penn State	MCL	AFM	Bruker
Penn State	MCL	AFM	Bruker
Penn State	MCL	AFM	Bruker
Penn State	MCL	AFM	Oxford Instrum
Penn State	MCL	White Light Interf...	Zygo

Implemented **browsing by instrument type** using a simple ontology.

Refined the Drupal plugin so that it can be **more easily updated** on partner installations, the **ontology of instrument types is dynamically populated** from the DMR-FIRST server, and the plugin can **mint DOIs** (via DataCite).

Implemented **instrument page validator** on [dmr-first.org](http://dmr-first.org) so web managers can check instrument web pages, especially those with institution-specific configuration.



**DMR-FIRST Instrument Tool**

**VALIDATE**

```
{
  category: "mbe",
  facility: "2DCC - 2D Crystal Consortium",
  @type: "ResearchInstrument",
  capabilities: "Up to 3" diameter substrates, adapter for (10x10)mm
  substrates, adapter for samples on Omicron T flag style holders
  Ultra-high vacuum shuttle for post growth characterization with up
  to 3 flag style holder sample storage capacity, base pressure 5x10-10
  Torr, equipped with a NexTorr pump keeping this vacuum for weeks
  without power supply
  Reflection high energy electron diffraction (RHEED) system 15kV,
  with RHEED analysis software kSA 400 version 5.50
  Spectroscopic ellipsometer, spectral range of 210-1690nm
  Residual gas analyzer for real-time background gas analysis
  Fully automated ion gauge beam flux monitor
  Fully automated heated quartz crystal monitor (room temperature
  to 500°C)
  Pyrometer for remote sample temperature measurements (in
  conjunction with in-situ spectroscopic ellipsometer)
  Chalcogenide reactor base pressure of 1x10-10 Torr
  Radio frequency plasma source to be used for oxygen, argon and
  nitrogen
  8 effusion cells (3 low temperature cells, 2 high temperature cells, 2
  dual temperature cells, 1 cracker cell)
```

### Errors

None

### Warnings

- *additionalProperty*: additionalProperty is recommended
- *purchaseDate*: purchaseDate is recommended
- *releaseDate*: releaseDate is recommended
- *model*: model is recommended
- *serialNumber*: serialNumber is recommended

### URL

None

## Development infrastructure updates

- Migrated to more recent build system (old build system no longer actively supported).
- Evaluated and selected front end testing framework, implemented first test cases.

# Mini-Workshop w/MRSEC Beta Testing Partners in May 2023

- Scheduled to accommodate MRSECs with reverse site visits in April.
- via Zoom, 90 minutes, recorded for anyone unable to attend.
- Illinois, UC Irvine, UC San Diego, UC Santa Barbara, Wisconsin (Princeton joined later).
- Included facility managers, web personnel, and leadership.
- Presented overview, tool demos, beta testing resources, support structure, next steps
- Plugin and documentation available to partners at password-protected [dmr-first.org](https://dmr-first.org).
- Followed up with one-on-one support calls with test partners.

## A major goal:



Test DMR-FIRST in diverse environments to identify pinch points and adaptations to ease broader adoption.

## Known unknowns:

- Need to increase compatibility with outdated versions of PHP.
- WordPress is more common than thought → **implemented Wordpress plugin**
  - **Same functionality as Drupal plugin** and independent of paid WP plugins.
  - Implemented instrument post type, JSON-LD metadata generation, view customization.

## Unknown unknowns, now known knowns:

- Penn State sites are administered by the materials community, but other some universities' sites are hosted by central IT, who may not authorize plug-in installation unless requested by a federal agency. **DMR-FIRST hosted mode (which doesn't require plugins) needs to handle these cases** without triggering central IT concerns around security/maintainability.
- The web presence for facility-level instrumentation is sometimes plain HTML (i.e. without a content management system) even when the main Center has a content management system. **DMR-FIRST hosted mode needs to scale simply and cleanly to handle multi-instrument sites** (it was originally envisioned to handle only single-PI instruments).

# Status of activities proposed in early/mid 2023 for completion by mid-2024...

## ✓ **Automation to conserve time of DMR-FIRST staff**

- Retrieve geolocations of buildings automatically
- ✓ DMR-FIRST server mints draft DOIs “within” institutional CMS
- ✓ More automated major instrument updates requiring new DOIs

✓ : **complete**

✓ : **in-progress**

## ✓ **CMS plugin for WordPress**

## **DMR Award Import Tool** to identify and reach out to new or existing instrument awardees

## ✓ **DMR-FIRST Hosted Mode** for instrument PIs without institutional facility websites

- ✓ Integrate with Shibboleth (single sign-on) so that hosted-mode users can log in using existing academic accounts
- ✓ Instrument editing framework identified, not yet implemented.
- ✓ Implementing hosted mode for PSU MRSEC instrumentation that is outside the Materials Characterization Lab.

## ✓ **Outreach to potential user community**

- A second virtual workshop targeting new users (e.g. MRI awards in the last X years, other national facilities)
- ✓ Refine instrument-type ontology and plug-in functionality, as informed by an expanding community of users
- ✓ Installation of DMR-FIRST plugin on partner test sites



# Looking ahead...

## On track with tasks proposed last year for completion by mid-year:

- The main remaining proposed tasks are finishing hosted mode, finishing work with test partners, holding a broader community workshop, and building an award import tool.

## New tasks identified through work with test partners:

- Hosted mode needs to be enhanced to handle larger sites that don't use a content management system and sites whose IT support has a restrictive plugin policy.
- Also, produce documentation to submit to IT to meet their requirements.

Scheduling of a **broader community workshop** should occur after implementation of the enhanced hosted mode and other items identified in beta partner interactions.

We also discussed DMR-FIRST (and LiST) with Bob Hanisch at NIST and Eva Campo, and **NIST is interested in visiting Penn State to explore partnerships.**