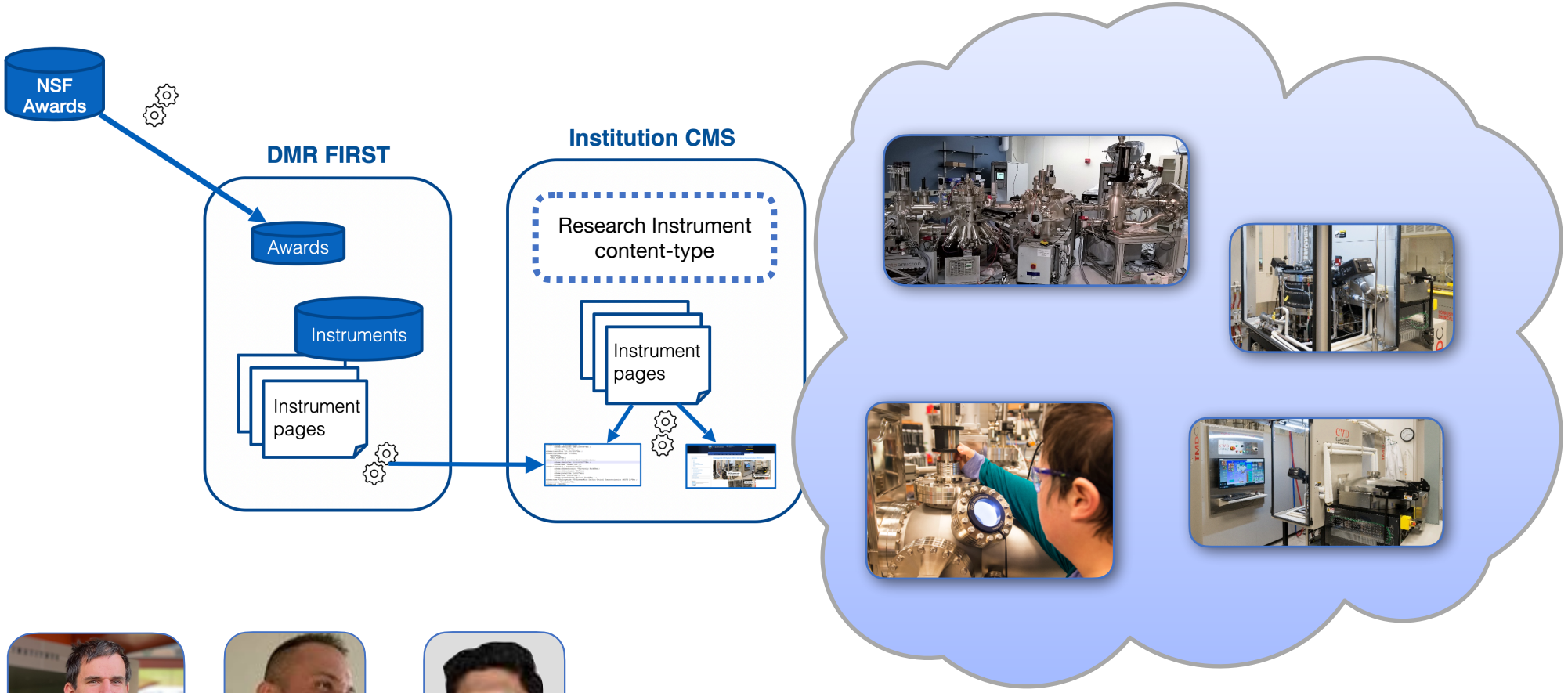
DMR FIRST Update

2D Crystal Consortium
NSF Materials Innovation Platform



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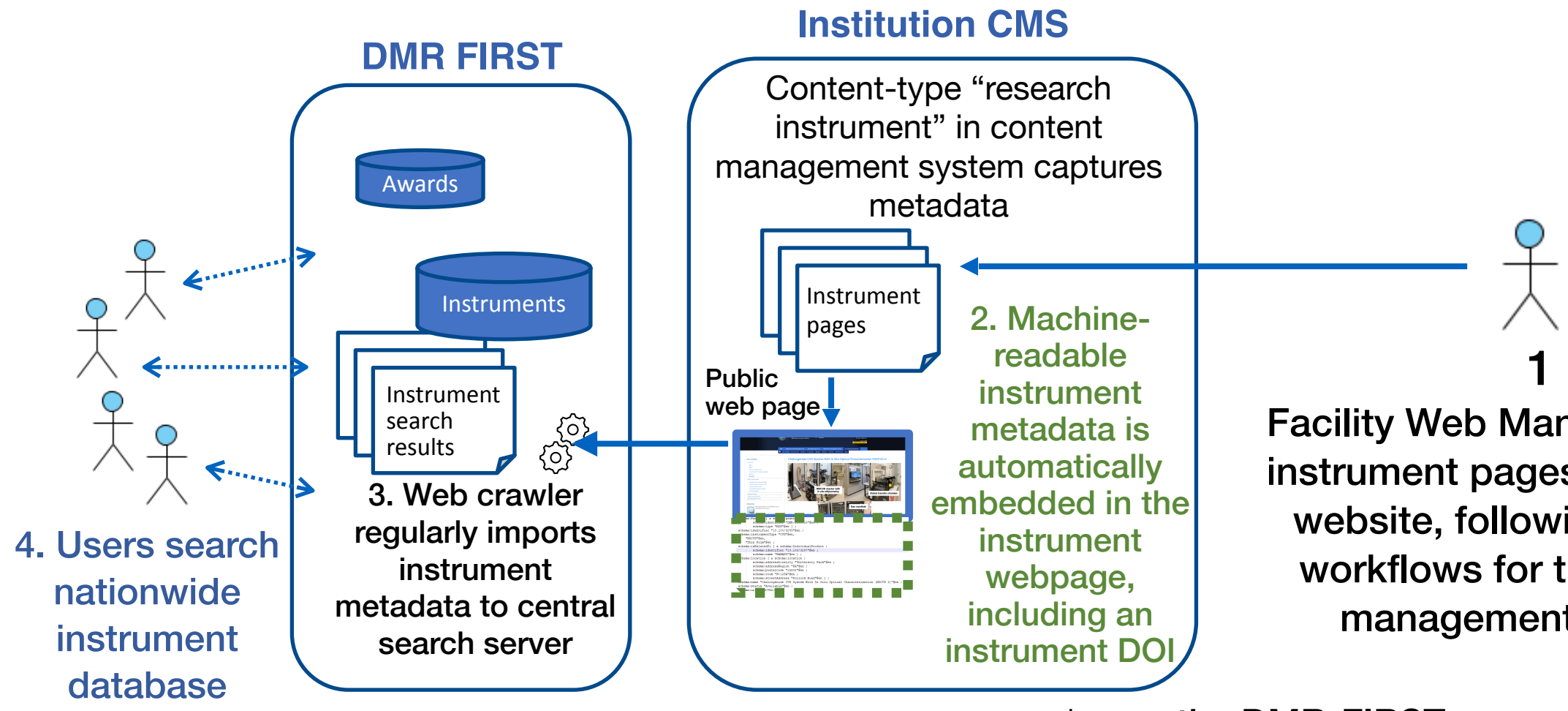
MRSEC Directors Meeting, February 2024

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.

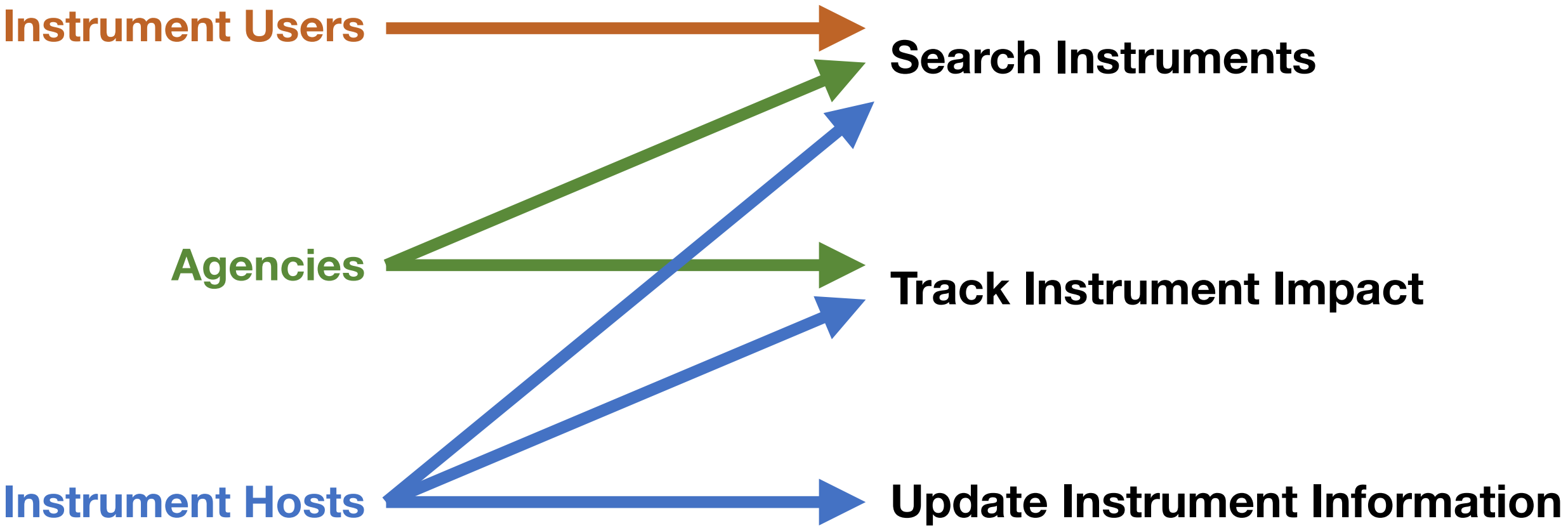


*or on the DMR-FIRST server, in hosted mode.

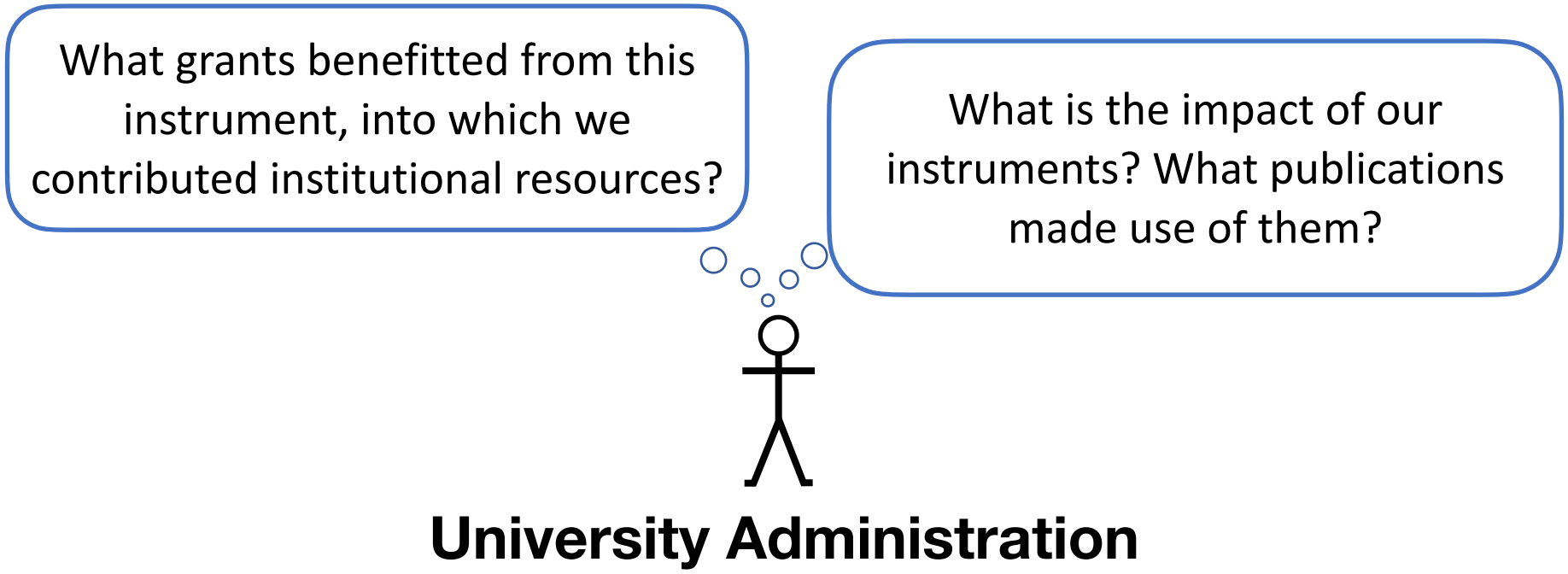
A federated database of DMR-supported instruments

- 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

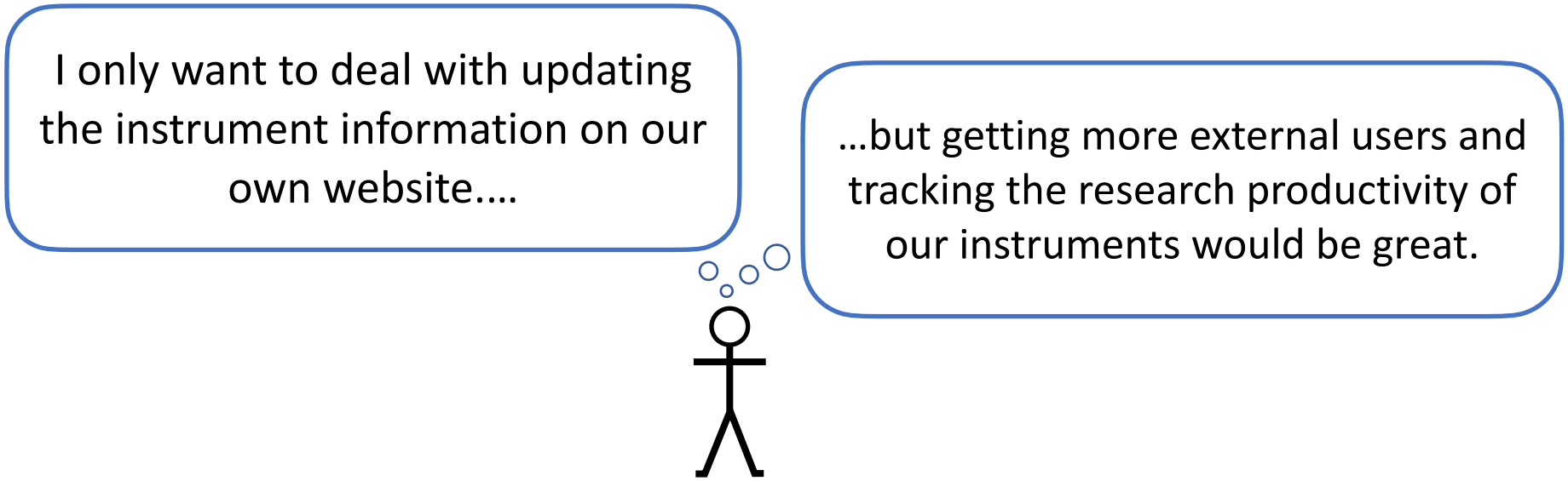

Instrument Users
Agencies
Instrument Hosts
Search Instruments
Track Instrument Impact
Update Instrument Information

Instrument Hosts



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

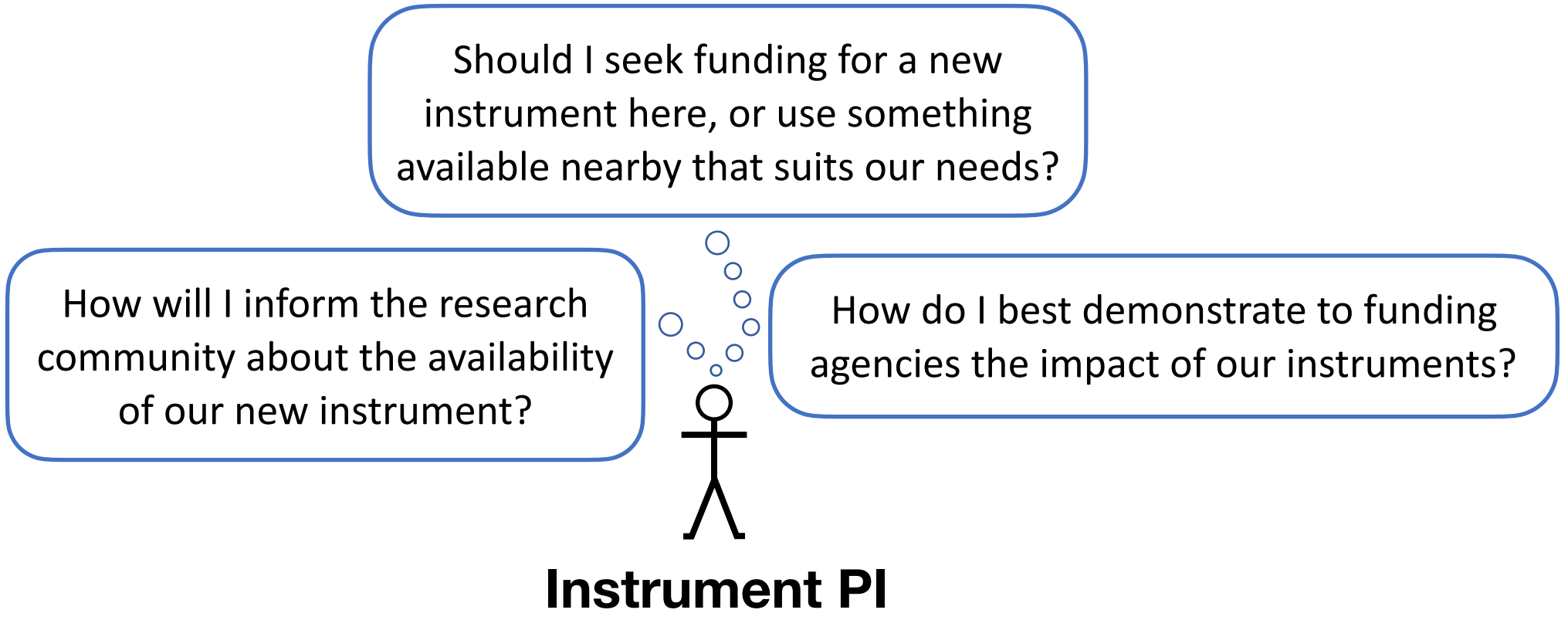
Instrument Hosts



Facility Manager, DMR Center/Platform Director

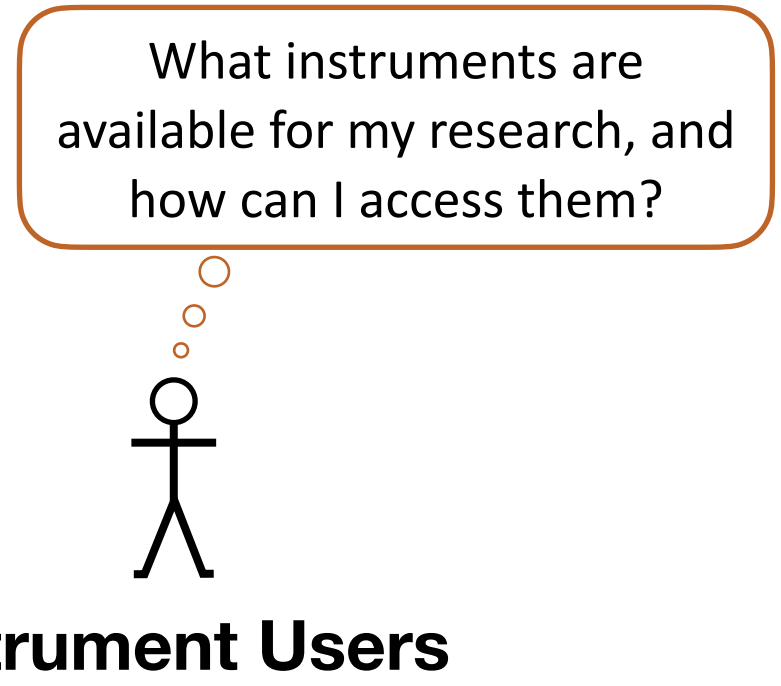
- Manage instrument data within existing content management systems with a DMR-FIRST plugin that can be styled by web managers.
- Instrument DOIs in publications document instrument impact.

Instrument Hosts



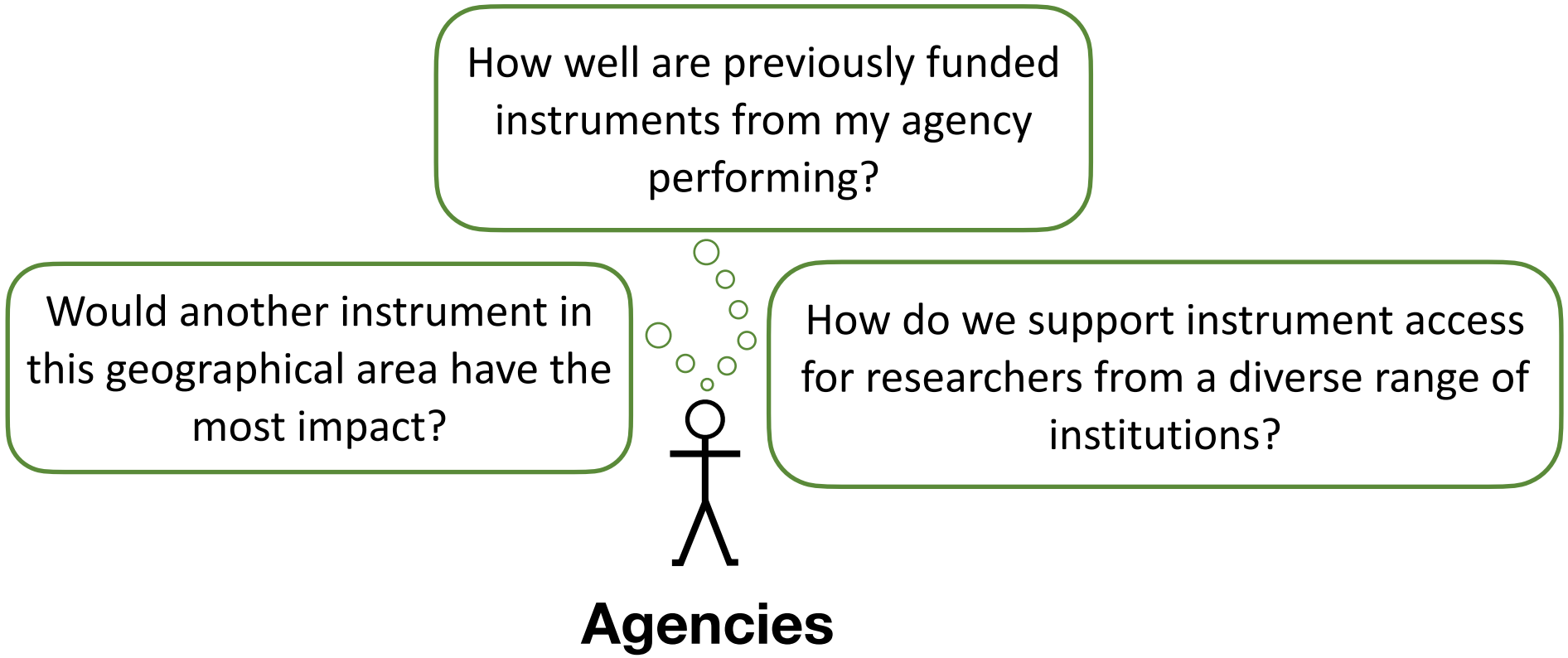
- Pre-award, instrument discovery informs whether to seek new instrument funding and helps make the case that one can secure a broad base of instrument users.
- Post-award, DMR-FIRST can provide a webpage (in the institutional context) as the instrument's public face without additional burden on local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

Instrument Users



- 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

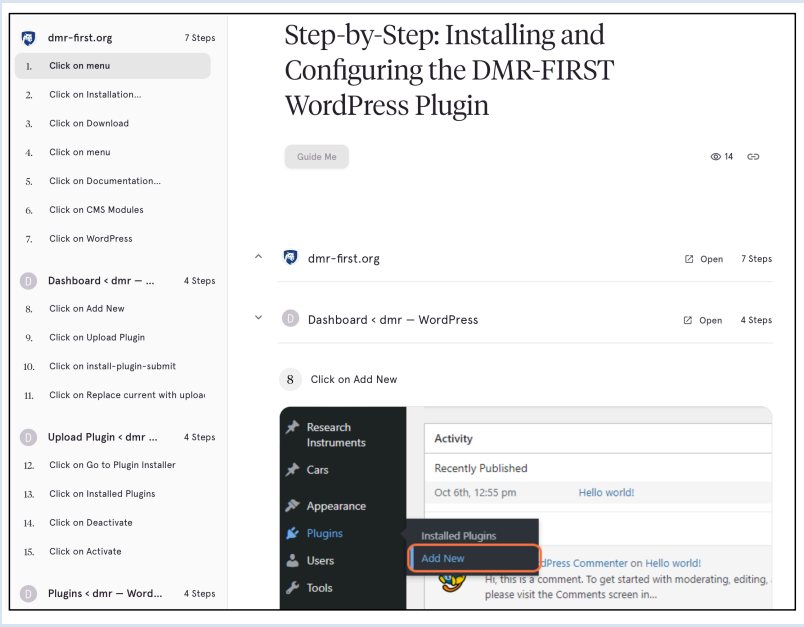


- DMR FIRST can increase awareness and access to instruments, and enable analytics of instrument interest, distribution, use, and impact.

Updates

Launched password-accessible dmr-first.org

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



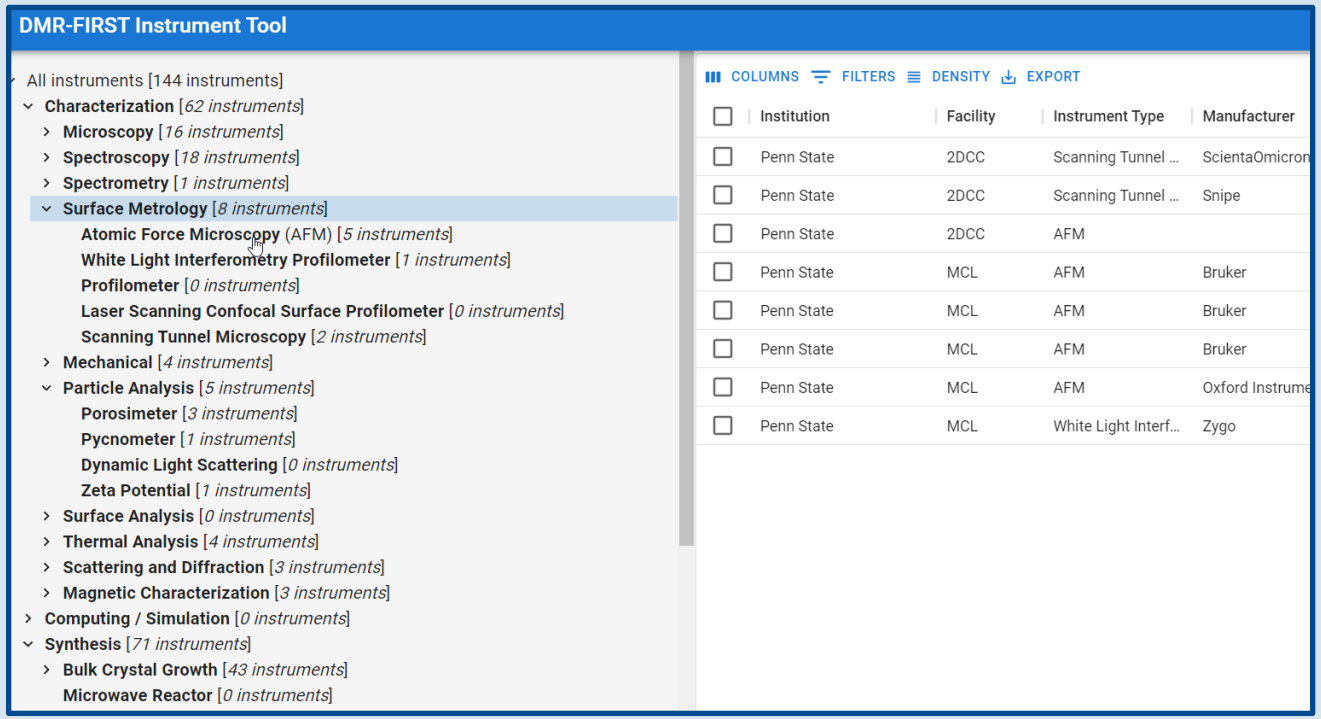
Updated Drupal module to support versions 9 & 10

- 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.

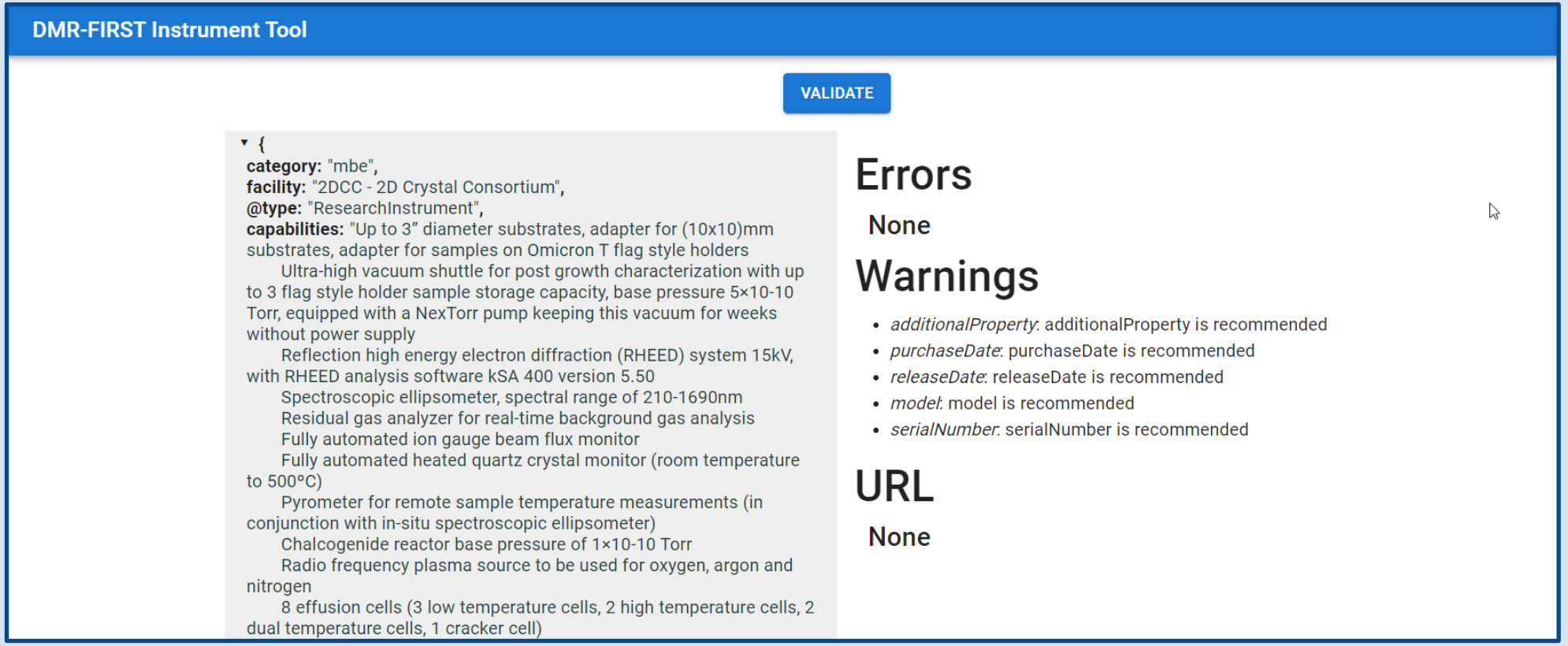
Implemented **linked instruments** (i.e. cluster tools), **instrument version control** for major (new-DOI) and minor updates of functionality, and an administrative interface on the DMR-FIRST server for database management.



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 so web managers can check instrument web pages, especially those with institution-specific configuration.



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.
- 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…

✓ **: complete**

✓ **: in-progress**

✓ 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

✓ 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**.