MICCoM

MIDWEST INTEGRATED CENTER FOR COMPUTATIONAL MATERIALS

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Headquarters at Argonne National Laboratory

Participants: University of Chicago, Northwestern University, University of Notre Dame, University of Michigan, University of California, Davis

http://miccom-center.org

Funded for 4 years, 3M/year, starting on Oct.1st, 2015

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OUTLINE

- The Center in a nutshell
- Three-task structure
  - Software
  - *Validation*
  - Data
- Conclusions

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MIDWEST INTEGRATED CENTER FOR COMPUTATIONAL MATERIALS

MICCoM develops and disseminates interoperable **open source software, data, simulation templates and validation procedures**, enabling the community to simulate and predict properties of functional materials for energy conversion processes. Emphasis is on heterogeneous materials, including defects and interfaces, the transport across them, and the manipulation of matter under conditions far from equilibrium.

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MICCoM'S DESIGN PRINCIPLES

- Equilibrium properties are not sufficient and may not be relevant to the design of new materials. New functionalities may arise in metastable systems
  - **Simulate and validate assembly processes occurring during synthesis**

- Functionality from building blocks (e.g. nanoparticles)
  - **Design building blocks with targeted properties**

- Design of heterogeneous systems
  - **Control of interfaces and defects**

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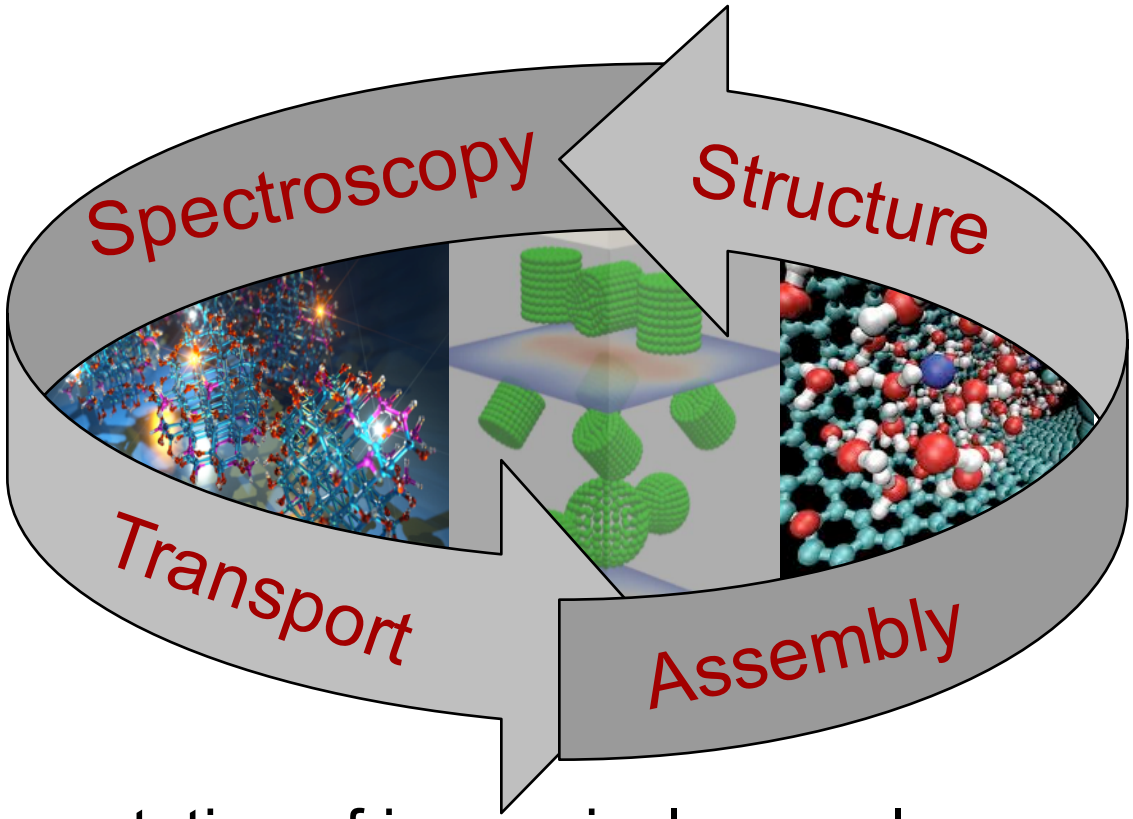
INTEGRATED MODELING OF MULTIPLE PROPERTIES



- Provide interpretation of increasingly complex experiments and provide validation of theory
- Determine & control: structure ←→ function
- Data analysis and optimization for rational design

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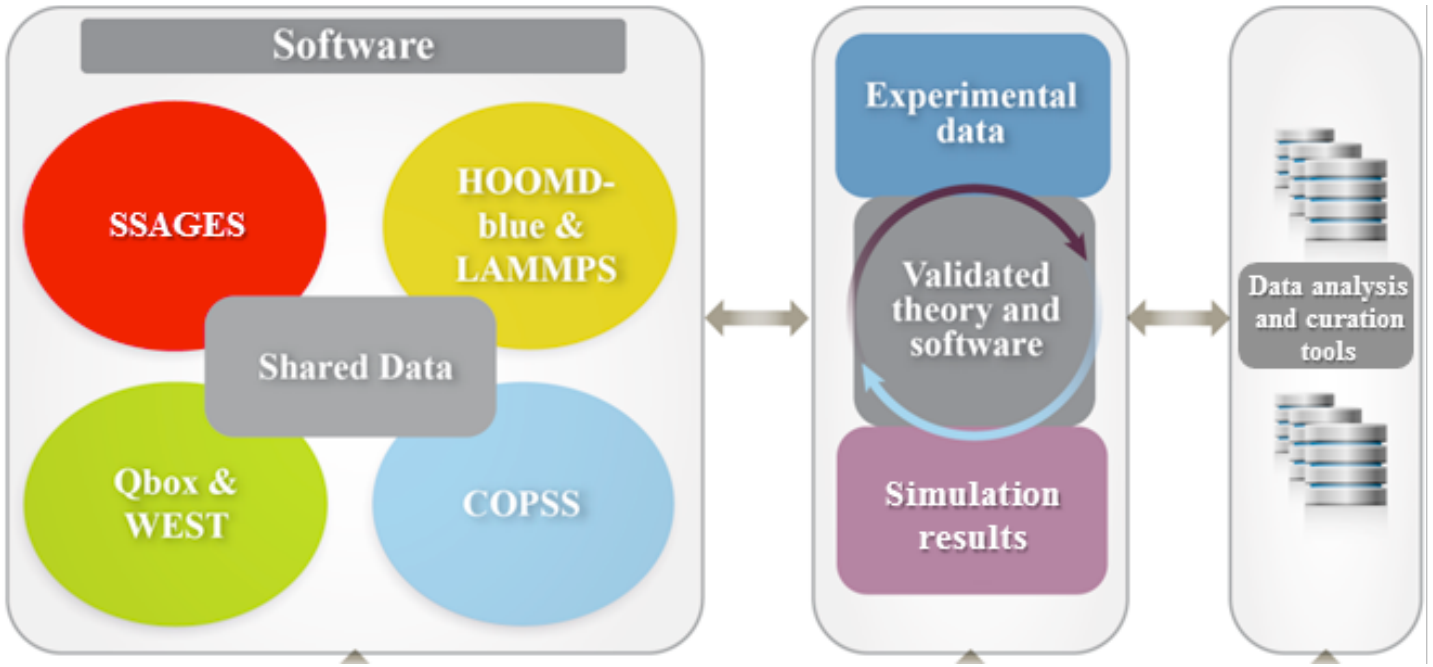
INTEGRATED CODES FOR DIFFERENT LENGTH SCALES AND MULTIPLE PROPERTIES



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MAIN OBJECTIVES OF THE SOFTWARE TASK

- Coordination of the software development between the maintainers of the four contributing software packages: SSAGES/COPSS, Qbox, WEST and HOOMD-Blue

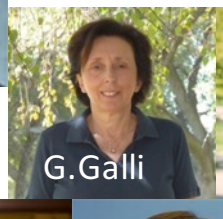
- Development of additional software for interoperability between the software packages

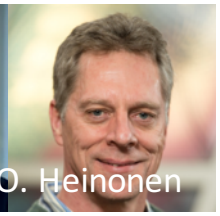
- Development of post-processing software for the analysis of molecular dynamics trajectories, spectroscopic data and transport properties (in collaboration with the Data Task)

- Optimization of the simulation codes for high-performance architectures

VERTICAL GROWTH FOR ADDED FUNCTIONALITIES & HORIZONTAL INTEROPERABILITY

- **Qbox**
  - First-principles MD (F.Gygi) http://qboxcode.org
- **WEST**
  - GW, BSE (M. Govoni, G. Galli) http://www.west-code.org
- **SSAGES/COPSS**
  - Advanced sampling and particle-continuum codes (J. de Pablo, J. Whitmer) http://ime-code.uchicago.edu
- **HOOMD-blue**
  - Classical MD (S. Glotzer, J. Anderson) https://codeblue.umich.edu/hoomd-blue
- ***LAMMPS*** *(used, not developed)*
  - *Classical MD (S. Plimpton) http://lammps.sandia.gov*





All codes open-source (GPL or modified BSD licenses)

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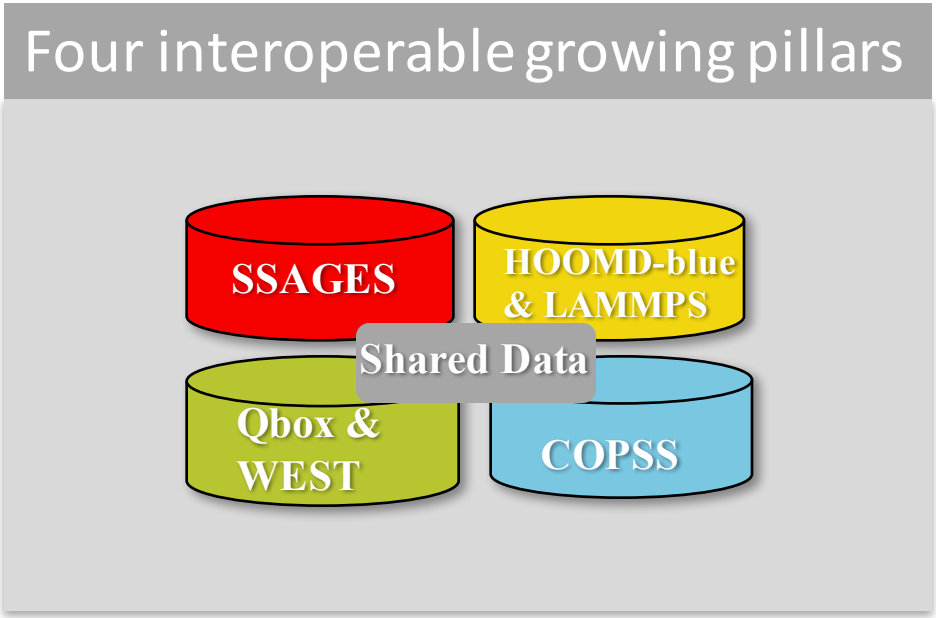

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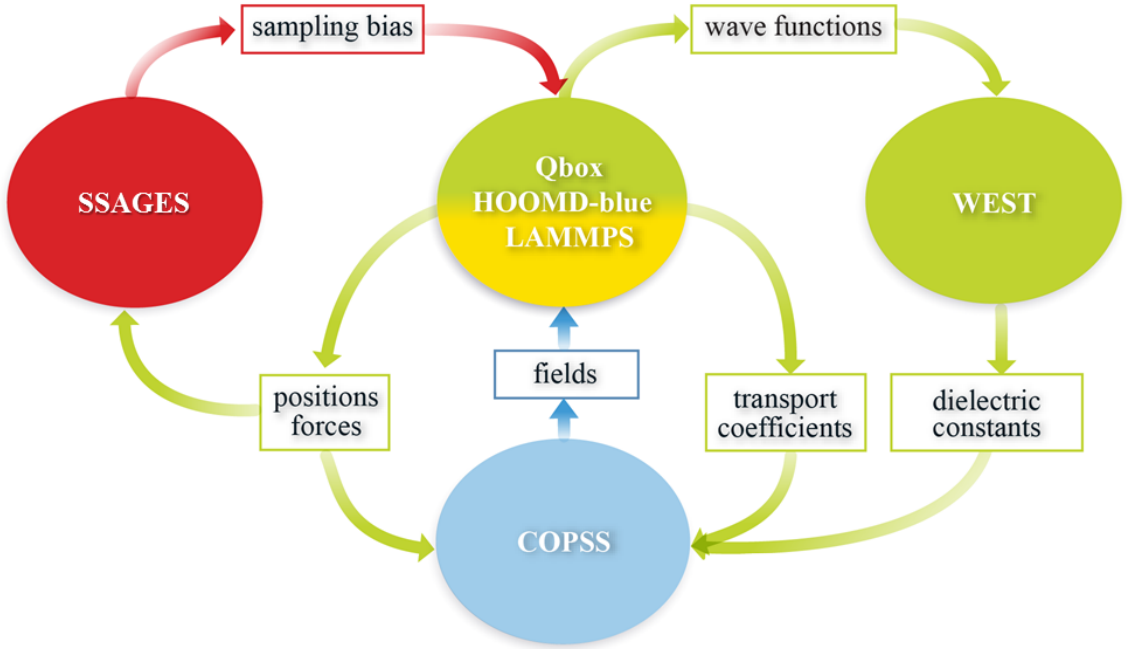
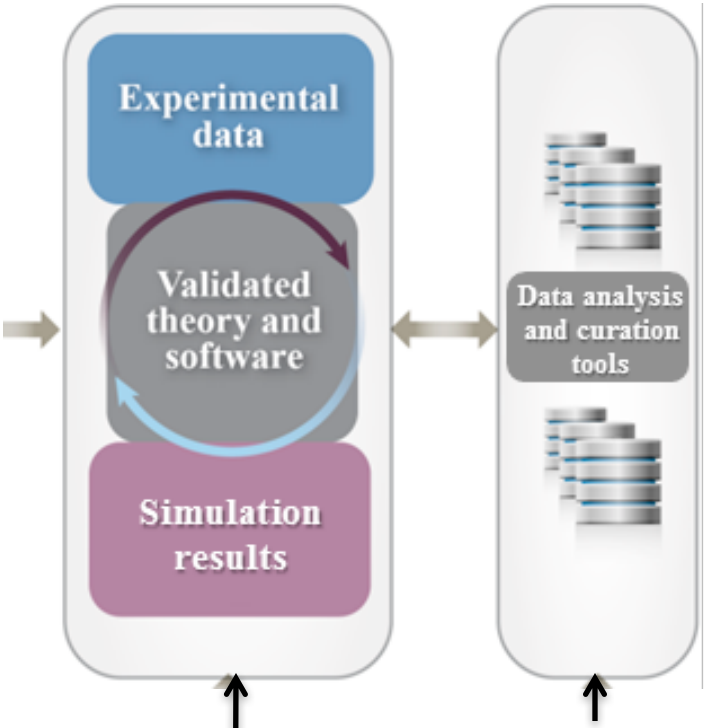
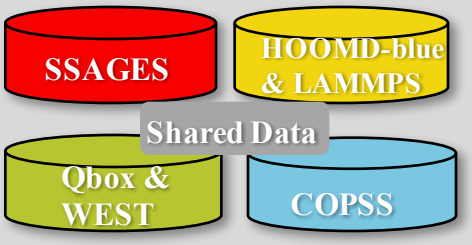




Four interoperable growing pillars



Re-use, analyze

Validate & control

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DATA TASK FOCI: PRODUCTION, COLLECTION, ANALYSIS

Three types of data to start with:

- MD trajectories:

http://www.quantum-simulation.org/reference/index.htm (ab initio); http://ime-code.uchicago.edu and https://glotzerlab.engin.umich.edu/signac (classical)

- Spectroscopic data: http://www.west-code.org

- Scattering data on ANL servers (set up in progress)

Pointers to available data: http://miccom-center.org/data.html

EXAMPLE: FPMD TRAJECTORIES

quantum-simulation.org

Home

Reference Data

Water PBE400 dataset

The water PBE400 dataset contains ab initio MD simulations of 32 independent 64-molecule water samples. A simulation consists of 120 runs of approximately 0.5 ps each, amounting to a total simulation time of approximately 58 ps for each sample. Samples are labeled s0000-s0031. Runs are labeled md001-md120. The cumulative simulation time is 32 * 58 ps ~ 1.86 ns. Equilibration time is included in the dataset.

Kohn-Sham energy

Kohn-Sham energy averaged over 0.5 ps interval

Velocity power spectrum

Power spectrum of atomic velocities

gOO(r) data

gOO(r) pair correlation functions

MD simulation data

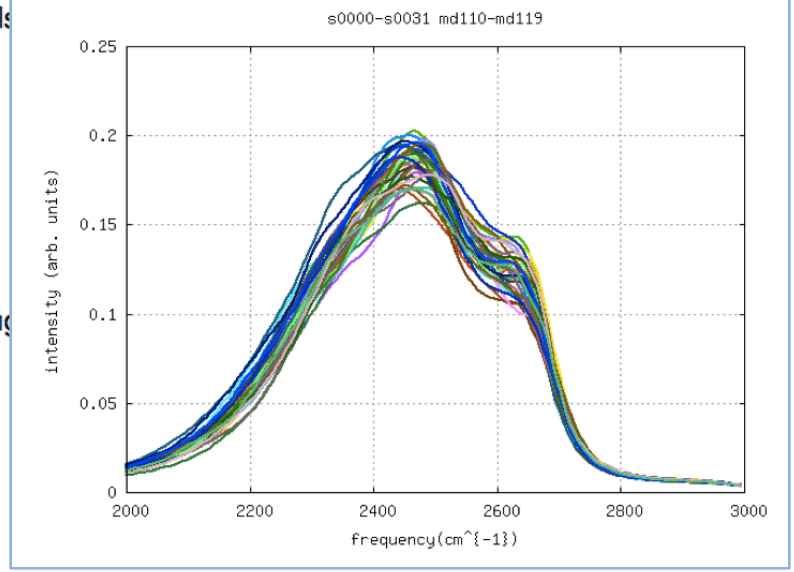
MD output files and xyz trajectory files

Restart files

Restart files containing the first <atomset> confi

Qbox load command).

D_2O power spectrum in the range of OH stretch frequencies.



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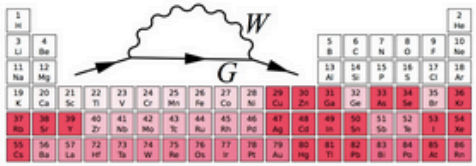
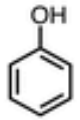
EXAMPLE: SPECTROSCOPIC DATA

WEST Database



WEST Database / GW100

Grid view

 Ethylbenzene (C_8H_{10})	 Ozone (O_3)	B≡N Boron Nitride (BN)	 Butane (C_4H_{10})	 Toluene (C_7H_8)
 Phenol (C_6H_6O)	 Pyridine (C_5H_5N)	 Tetracarbon (C_4)	P≡P Diphosphorous (P_2)	Ag—Ag Silver Dimer (Ag_2)
Cu—Cu Copper Dimer (Cu_2)	O=C=O Carbon Dioxide (CO_2)	Be=O Beryllium Monoxide (BeO)	Mg=O Magnesium Monoxide (MgO)	 Borane (BH_3)
H—H Dihydrogen (H_2)	B—F Boron Monofluoride (BF)	Li—Li Lithium Dimer (Li_2)	 Pentasilane (Si_5H_{12})	 Disilane (Si_2H_6)
 Carbon Monoxide Selenide (COSe)	Ga—Cl Gallium Monochloride (GaCl)	P≡N Phosphorus Nitride (PN)	 Diborane (B_2H_6)	As≡As Diarsenic (As_2)
Na—Na Sodium Dimer (Na_2)	K—K Potassium Dimer (K_2)	Rb—Rb Rubidium Dimer (Rb_2)	 Hydrazine (N_2H_4)	 Hexafluorobenzene (C_6F_6)
Sodium Tetramer (Na_4)	Sodium Hexamer (Na_6)	 Carbon Monosulfide (CDS)	 Formaldehyde (CH_2O)	 Carbon Tetraiodide (CI_4)
 Cyclopentadiene (C_5H_6)	 Cu—C≡N Copper Monocyanide (CuCN)	 Carbon Tetrabromide (CBr_4)	 Carbon Tetrachloride (CCl_4)	 Urea (CH_4N_2O)

EXAMPLE: SPECTROSCOPIC DATA

System details

Compound	Pyridine
Formula	C_5H_5N
CAS Number	110-86-1

Ground state input	**Values**
Cubic cell size	15 Å
PW cutoff (WFS)	55 Ry
Pseudopotential	SG15[01]

HOMO (Highest Occupied Molecular Orbital)

Level	Software	Details	Energy (eV)
G_0W_0@PBE	BerkeleyGW[02]	GPP	9.5
G_0W_0@PBE	BerkeleyGW[02]	FF	
G_0W_0@PBE	FHI-aims[02]	2P	9.08
G_0W_0@PBE	FHI-aims[02]	16P	9.04
G_0W_0@PBE	FHI-aims[02]	extrapolated	9.17
G_0W_0@PBE	Turbomole[02]	RI	9.01
G_0W_0@PBE	Turbomole[02]	no-RI	
G_0W_0@PBE	**WEST[03]**	**1-shot**	**9.27**
G_0W_0@PBE	**WEST[03]**	**secant**	**9.13**
G_0W_0@PBE	**WEST[03]**	**plot**	**xxxx**
CCSD(T)	Turbomole[04]	def2-TVZPP	9.659
EXP.[05]			**9.51***

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DISTRIBUTED DATA

Pointers to NIST repositories to make data **searchable** (https://materialsdata.nist.gov); MICCoM community defined (https://materialsdata.nist.gov/dspace/xmlui/community-list) to make data **discoverable**

MD trajectories

Spectroscopic Data

Scattering Data

Data on servers running NIST curator to make data **interoperable**

Globus end points

https://www.globus.org/

Analysis codes on same servers and/or downloadable from MICCoM Wiki (in progress) and software URLs

https://materialsdata.nist.gov/dspace/xmlui/

NIST Repositories

Communities in NIST Repositories

Select a community to browse its collections.

- ASM Structural Materials Data Demonstration Project
- Bell Test Data
- CHiMaD Data Collections
- Computational File Repository
- Experimental Data Repository
- Genome in a Bottle
- Heusler Phases: First Principles Simulations
- ICME Approach to Development of Lightweight 3GAHSS Vehicle Assembly
- ICME of Carbon Fiber Composites for Lightweight Vehicles
- MGI Catalogs
- MICCoM Collections
- NanoRelease
- NIST/DOE-EERE Advanced Automotive Cast Magnesium Alloys
- NIST Thermodynamics and Kinetics Test Space

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The National
DATA SERVICE

Home About Projects News Get Involved

Home > Projects > The Materials Data Facility

The Materials Data Facility

The Materials Data Facility (MDF) is a scalable repository where materials scientists can publish, preserve, and share research data. The repository provides a focal point for the materials community, enabling publication and discovery of materials data of all sizes.

MDF is a pilot project funded by NIST, and serves as the first pilot community of the National Data Service.

Materials Data Curation System

https://mgi.nist.gov/materials-data-curation-system

DESCRIPTION:

The NIST Materials Data Curation System (MDCS) provides a means for capturing, sharing, and transforming materials data into a structured format that is XML based amenable to transformation to other formats. The data are organized using user-selected templates encoded in XML Schema. These templates are used to create data entry forms. The documents are saved in a non-relational (NoSQL) database, namely MongoDB. The data can be searched and retrieved via several means: by a template-driven web-based form, by a SPARQL endpoint query, and by a RESTful API call. The system also enables the interconnection of MDCS repositories for federated searches.

MAJOR ACTIVITIES:

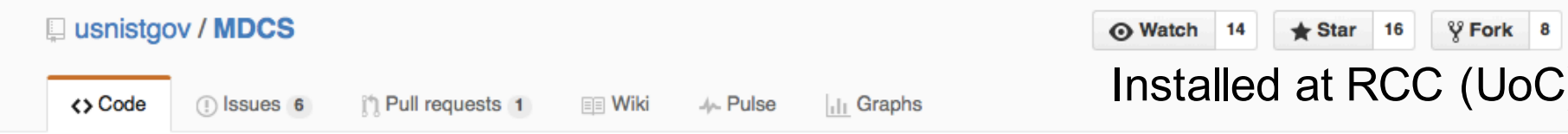
We have had five releases in 2015. These releases included an XML Schema composer to allow for rapid development of XML schemas for reusable types, a new UI module system that allows for fully featured applets to be associated with XML tags, implementation of new administrative features such tools to perform repository back up and restoration, implementation of stored XML document editing allowing for full round trip processing of data stored in the repository, and a number of enhanced XML tools and features. The latest versions added the ability to compose XML schemas from smaller schemas which represent highly reusable types and the ability to store images and other Binary Large Objects (BLOB). The MDCS is available from https://github.com/usnistgov/MDCS.

PRESENTATIONS AND RELATED DOCUMENTS:

usnistgov / **MDCS**

Watch 14 | Star 16 | Fork 8

Installed at RCC (UoC)



Materials Data Curation System

73 commits | 3 branches | 6 releases | 2 contributors

Branch: **stable** | New pull request | New file | Find file | HTTPS | https://github.com/usnist | Download ZIP

Guillaume-sousa Fix Issue Exporters / API select template — Latest commit 5824e85 17 days ago

admin_mdcs	Version 1.3	3 months ago
api	Fix Issue Exporters / API select template	17 days ago
bin	Version 1.2	7 months ago
compose	Version 1.3	3 months ago

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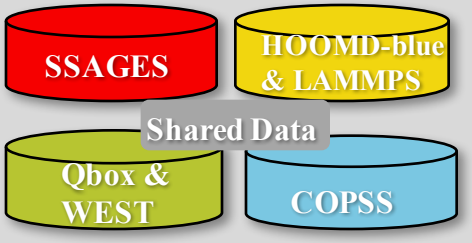

http://miccom-center.org

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Argonne NATIONAL LABORATORY

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NORTHWESTERN UNIVERSITY

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