ROYAL INSTITUTE OF TECHNOLOGY

Project 2019 – AM-database

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THE SWEDISH ARENA FOR AM OF METALS

Outline

- Aim of proposed project
- Configurational Data Curation System (CDCS)
- Project work packages and time plan

2019 Technical Group Project

***Aim**: Capture and store AM-related materials data produced within PhD/postdoc projects at Swedish universities in an open searchable and reusable structure.*

Motivation

- Materials science is becoming more data intensive
- Data-driven techniques (e.g., machine learning) are becoming more common
- Awareness and education

2019 Technical Group Project

***Aim**: Capture and store AM-related materials data produced within PhD/postdoc projects at Swedish universities in an open searchable and reusable structure.*

Approach

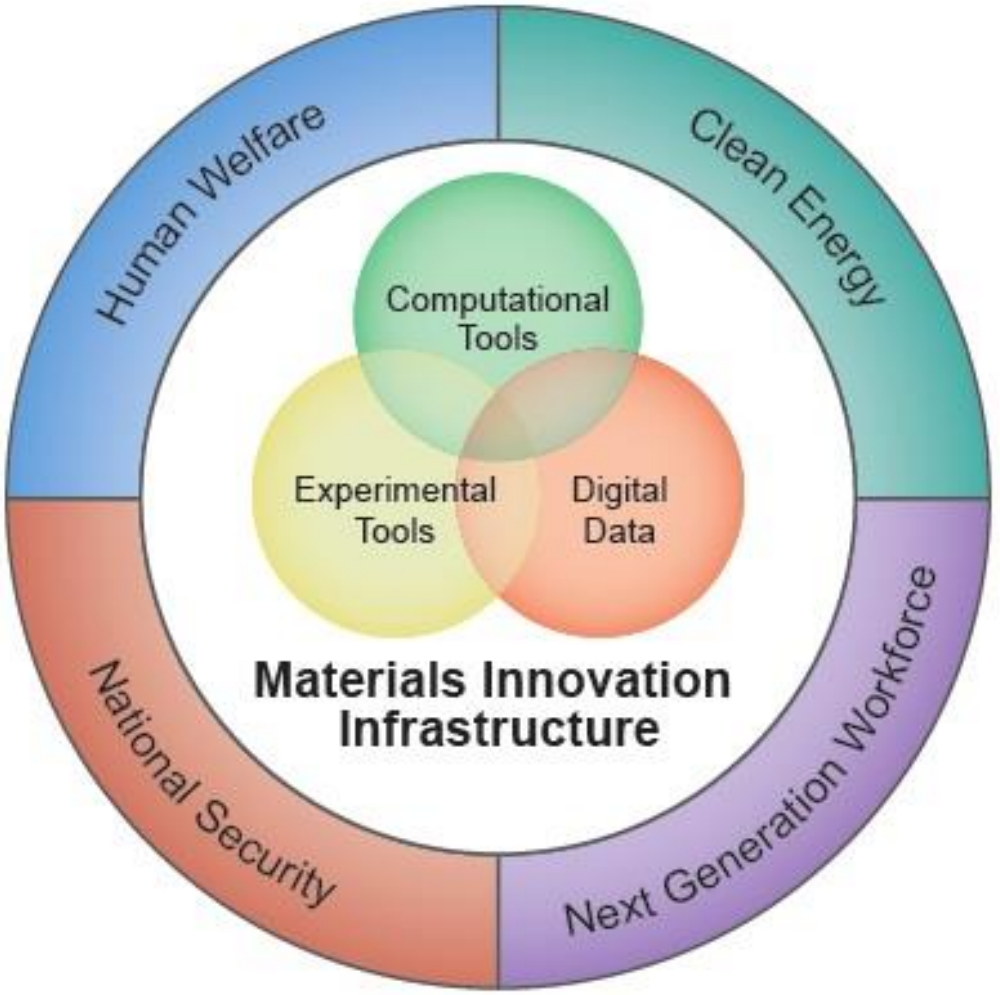
- Make use of available materials data infrastructures (suggestion: to use CDCS)
- Setup a common repository/database
- Train students in using CDCS to fill the repository
- Engage students in collaborative activities

Materials Genome Initiative (MGI)

A U.S. multi-agency initiative to create policies, resources and infrastructure to support

- Discovery
- Manufacturing
- Deployment

of advanced materials twice as fast and at a fraction of the cost.



Holdren, MGI for global competitiveness (2011)

MGI activities at NIST

General Info:

- NIST MGI: MGI.NIST.GOV
- Center for Hierarchical Materials Design: chimad.northwestern.edu

Software

- Materials Data Curation System: https://github.com/usnistgov/MDCS
- Materials Resource Registry: https://github.com/usnistgov/MaterialsResourceRegistry
- Materials Design Toolkit: https://mgi.nist.gov/materials-design-toolkit
- Cloud of Reproducible Records: https://mgi.nist.gov/cloud-reproducible-records

Data Resources

- Materials Resource Registry (tool to search for resources): materials.registry.nist.gov
- Schema Registry: Schemas.nist.gov
- MaterialsData Repository (General Materials Data): materialsdata.nist.gov/
- Phase-based Data Repository: PhaseData.NIST.GOV
- Interatomic potentials: www.ctcms.nist.gov/potentials/
- Density Functional Data: www.ctcms.nist.gov/~knc6/JVASP.html

National Institute of Standards and Technology
U.S. Department of Commerce

Configurable Data Curation System (CDCS)

- Need
  - Scientific data exists in many formats
  - Difficult to
    - Combine data from multiple sources
    - Understand and reuse existing data
    - Find associated metadata
    - Transform data into new formats
- Objectives
  - Facilitate collection, use, and reuse of materials data
  - Provide needed informatics infrastructure to enable High Throughput Experimentation (HTE)

https://github.com/usnistgov/MDCS

- Achievements and Impact
  - Made available to community via GitHub
  - Several early adopters of CDCS

Warren & Ward, JOM 2018:70

Overall Design - CDCS

GUI

Web Framework

REST API

Exporter

Digital Data & Metadata (any format)

Data Analysis Infrastructure

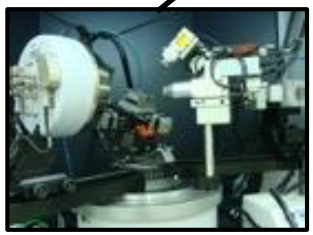
Simulation

User Scripts

Harvester

Data Provider

Data Management & Search Engine



Measurement

Data
Metadata

Database

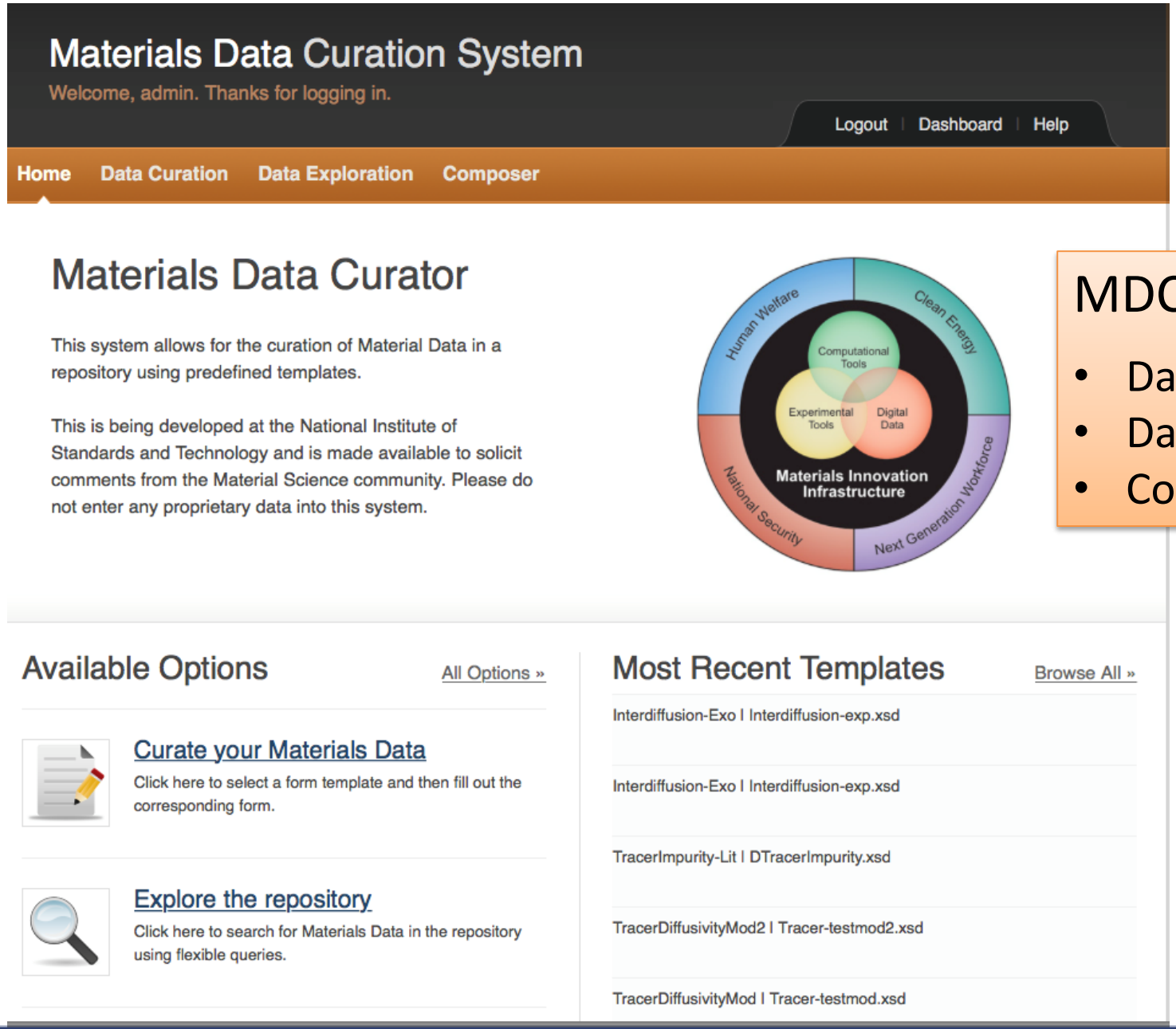
Images
Large Files
BLOBs

Large Dataset Repository

Data Provider

Harvester

https://github.com/usnistgov/MDCS



MDCS Functions

- Data Curation
- Data Exploration/Exporter
- Composer

Why use CDCS?

- Open-source software built on widely used open-source software packages (MongoDB, Django, Redis, Celery)
- XML format (text based) – readable by machines and humans
- It already has built-in APIs (very important!)
- It's available and it's developed for these purposes acknowledgeing
- It's been developed for years and is still being developed (XML schemas for AM)

Example: AM Bench Schema

Additive Manufacturing Benchmark test series

Its intent is to develop a continuing series of controlled benchmark tests + conference series

Main goals:

(1) Allow modelers to test their simulation results against rigorous and controlled experimental data

(2) Encourage AM practitioners to develop novel mitigation strategies of challenging build scenarios

Example: AM Bench Schema

AM-Bench 2018 measurements

1) Laser powder bed fusion (L-PBF) 3D builds of Ni-based superalloy IN625 and 15-5 SS test objects: modelers were challenged to predict the part deflection, residual elastic strains, microstructure, phase fractions and phase evolution.

2) Individual laser traces on bare metal plates of IN625 for different laser power and scanning speed: modelers were challenged to predict melt pool geometry, cooling rate, topography, grain shapes, dendritic microstructure and 3D structure.

3) Materials extrusion polymer 3D builds of test objects: modelers were challenged to predict part thickness, mass, tensile properties, void distribution and cross section.

4) Polymer powder bed fusion (P-PBF) with test objects being of dogbone shape and of Nylon 12: modelers were challenged to predict part thickness, mass, tensile properties, void distribution, cross section, crystallinity and melting.

www.nist.gov/ambench

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2019 Technical Group Project

Four workpackes

- WP1 – Setup
- WP2 – Organization
- WP3 – Training
- WP4 – Data capture

WP1 – Setup

Setting it all up at the host-university and write manual (API documentation). Explore required conditions for a sustainable solution.

Suggested tasks

1. Decide on host, set the design and name
2. Set up the main server and administer
3. Set long-term development
4. Set long-term funding

2019 Technical Group Project

Four workpackes

- WP1 – Setup
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WP2 – Organization

Coordinate the work. Nominate CDCS ”ambassadors” (PhD student/postdoc) at each university to lead the in-house CDCS activities and communicate the sub-group.

Suggested tasks

1. Nominate ambassadors
2. Project management
3. Follow and communicate the progress of the work

2019 Technical Group Project

Four workpackes

- WP1 – Setup
- WP2 – Organization
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WP3 – Training

Training of students in how to use CDCS, how to develop XML Schemas and use rest-API.

Suggested tasks

1. Hands-on workshops at the universities
2. Document rest-API function

2019 Technical Group Project

Four workpackes

- WP1 – Setup
- WP2 – Organization
- WP3 – Training
- WP4 – Data capture

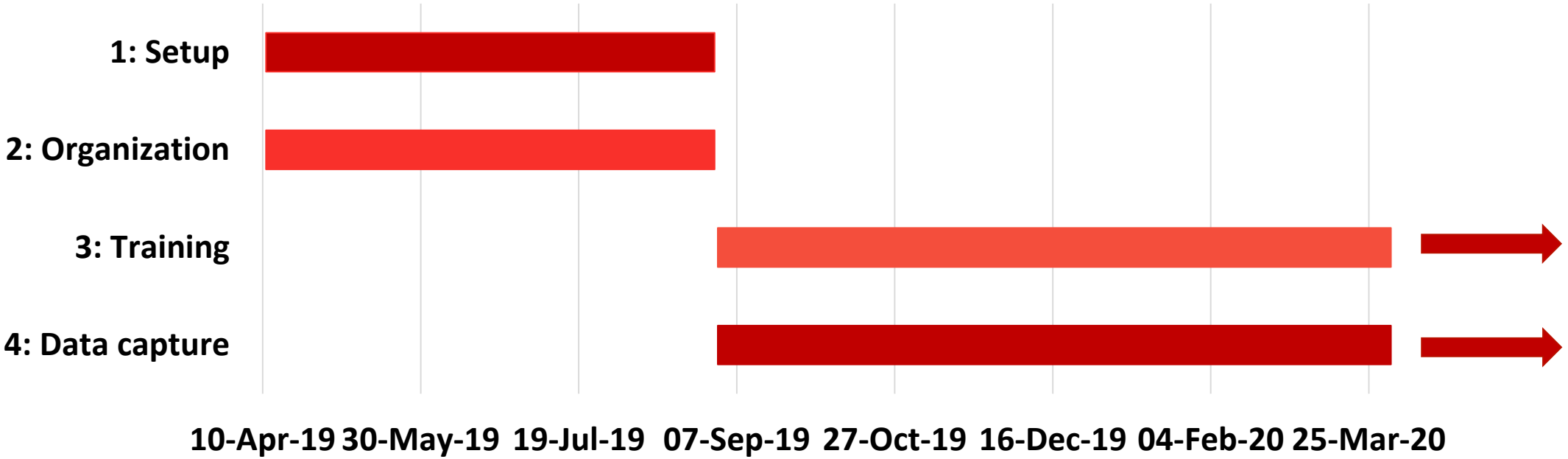
WP4 – Data capture

Data capturing and creation.
Engagement activites to accelerate the work, motivate the students and help reach consensus on common schemas temlates for similiar types of data sets.

Suggested tasks

1. Data capture and curation at each university
2. XML schema ”hackatons”

Time plan


1: Setup
2: Organization
3: Training
4: Data capture
10-Apr-19
30-May-19
19-Jul-19
07-Sep-19
27-Oct-19
16-Dec-19
04-Feb-20
25-Mar-20

https://amdata.proj.kth.se/