Project duration: 01.01.2023 - 31.12.2025

MSE - Material

Metals/Alloys: High-alloy steels (316L, Duplex ER2209)

MSE - Application areas

Process optimization: Improved welding based additive manufacturing by developing methodology to predict material−process−property relationships, so that simulations and machine learning can accelerate process optimization.

MSE - Product Lifecycle

Manufacturing: Improve Wire Arc Additive Manufacturing (WAAM) and Wire Laser Additive Manufacturing (WLAM).

MSE - Material properties

Mechanical: Measurements of hardness, Young's modulus.
Thermodynamic: Use of thermodynamic databases to predict phases and microstructure.
Crystallographic: Measurement and prediction of microstructure of welded samples.

MSE - Approach

Experiments: Manufactured standard sample geometries of 316L steel, analysed microstructure of samples in detail.
Computer Simulations: Simulations of process temperatures hence microstructure.
Machine Learning/Statistical/Big data: Analysis of correlations between process parameters and manufacturing outcomes to optimize process state.

MSE - Material scales

Mesoscale: Microstructure, grains, phases, concentrations
Continuum/Macro-scale: Thermal simulations

General - Centrality of FAIR

Findability: Using a triplestore database it is possible to search for material properties as a function of manufacturing parameters, and not just as a function of sample ID.
Accessibility: Data can be accessed via a web-based query interface (SPARQL REST API) or an interactive user interface (Vue.js).
Interoperability: Terminology differs between WAAM, WLAM and analytics experts. The process ontology helps communication.
Reusability: The data model is compatible with PMDco providing a common framework for reusability.

General - Types of data

Raw data: Sensor data (recorded during manufacturing process), characterization data (microstructure, phases etc.), images and videos.
Processed data: Output of process simulations.

General - Documentation and publishing of data

Field-specific data repositories: DiMad DB (web-based graph database)
General data repositories: Zenodo
Code repositories: GitHub
Other repositories: PMD Workflow Store
Other: Siemens Edge computer with Siemens data-acquisition app

General - Proprietary/Non-proprietary

Mostly proprietary data: Data from own laboratory tests in proprietary file format.

Ontologies - Aspects of digitalization

Procedures for ontology development: Development of a holistic WAAM / WLAM process ontology based on PMDco.
Data transformation using ontologies: Use ontologies to maintain knowledge while transforming data.
Publishing/disseminating knowledge graphs
LLM integration: Consider LLM as a natural language interface for web-based graph database.

Ontologies - Levels of structured data handled

Human-readable documentation: Jupyter Notebook, Word, Excel.
Partially structured data: Established data structures for process and characterization data.
Ontologically described data (RDF data): RDF data for process simulation and characterization.

Ontologies - Existing ontologies used

MSE ontologies: PMDco 2.0.7, MWO
Domain-specific ontologies: DiMad application ontology

Ontologies - Tools for ontologies

Editors and Collaborative tools: Protégé, Inforapid Knowledge Base Builder
Triple Stores and interfaces: Apache Jena Fuseki, OntoDocker
Formats and Languages: RDF, OWL, Turtle
Utility python libraries: CSV2RDF, RDFlib

Workflows - Types of workflows

Data acquisition from experiments: Characterization data - automated format translation from Word to C# and .NET. IR-camera, videos, scanned data, timeseries data (primarily WAAM) for current, voltage, wire feed and laser power.
Post-processing/analysis of raw data: Manual evaluation of characterized data.
Machine-learning: Under development; not yet clear how exactly the results of the machine-learning analyses are connected or fed back to other workflows.
Computer simulation pipelines: Process and microstructure simulations.

Workflows - Workflow priorities

Automation of workflows.
Better documentation.
Better reproducibility.

Workflows - Workflow challenges

Automation: Data transfer

Workflows - Levels of workflow implementations

Script jobs: Python, Bash
Pre-defined but extendible workflows: Jupyter Notebooks
User friendly interfaces for workflows: AixViPMaP
Interoperable workflows following community standards: pyiron

Workflows - Publishing of workflow-related elements

Complete workflows: Microstructure solidification simulation of 316L steel during WAAM
Software packages: pyiron_micress implementing MicressJob

Workflows - Use of PMD workflow store

Publish own workflows/modules: MICRESS simulation including post-processing with MicPy.

Workflows - Tools for workflows

Workflow management: AixViPMaP, pyiron, PBS
Simulation/CAD tools: MICRESS, Thermo-Calc, NX (NX Open API), Ansys (ACT)
Analysis visualization tools: ParaView/VTK, DP_MICRESS, Jupyter Notebook
Experimental software: Siemens data-acquisition app
Utility python Libraries: numpy, pandas, matplotlib, micpy, docx
Tools for ontologies/RDF data: rdflib, Protégé
ML/LLMs: AutoEncoder, FeedForwardNetwork, AutoML, Image Processing

IT & Security - Computational demands

Local workstation: Thin client
Usage of HPC resources: PBS
Usage of cloud resources: AWS, ownCloud, NextCloud

IT & Security - Data-federation

Within own institution: Object storage (Kibana, ElasticSearch, S3).
With project partners: Cloud storage (ownCloud, NextCloud), graph database (Apache Jena).
PMD-S: AixViPMaP (SSO via PMD-S).

IT & Security - Software user interface

Web-service (GUI): AixViPMaP
Web-service (API): File management (WebDAV), QR code generator (FastAPI)
Executable: PyData Stack
Desktop app: MICRESS, Thermo-Calc, ParaView

IT & Security - Data encryption

Encryption: SSL/TLS
Certification: SSL/TLS

IT & Security - Tools for IT-architecture and security

Containerization tools: Docker, Compose
AAI (auth & access infra) tools: Custom tools (e.g. SSH wrapper)
Operating systems: Windows, Ubuntu
Data sharing tools: WebDAV (e.g. NextCloud client)
Data back-ends: S3

Use of PMD-Tools

Workflowstore   **PMDco**   **pyiron**   **PMD-S**