Development of a User-Friendly Virtual Material Characterization Toolbox

A Data Management Plan created using DMPonline.be

Creators: n.n. n.n., Martin Diehl, Ward Melis, Stijn Schildermans

Affiliation: KU Leuven (KUL)

Funder: KU Leuven (KUL)

Template: KU Leuven BOF-IOF

Principal Investigator: Stijn Schildermans

Project Administrator: n.n. n.n., Martin Diehl, Ward Melis

Grant number / URL: C3/23/053

ID: 205276

Start date: 01-07-2024

End date: 30-06-2026

Project abstract:

Metal parts used in high-value applications need to fulfill strict requirements with respect to accuracy and mechanical properties. Integrated computational tools are essential to develop such parts efficiently. These tools aim to predict mechanical behavior by modeling metal alloys as polycrystals, in which each grain has a distinct orientation. The distribution of these orientations is responsible for the anisotropy typical for many metals. Said anisotropy is altered throughout the production process. KU Leuven developed a tool to simulate this evolution during the forming process, called ALAMEL/VEF. While proven to provide excellent simulation results, this tool is currently only suited for academic use, lacking many features essential to a pleasant user experience such as a graphical user interface and the ability to visualize input and output data. This project aims to provide precisely this, building a web-based framework around the existing tool so that materials engineers may effortlessly perform simulations and process results.

Last modified: 06-03-2024

Development of a User-Friendly Virtual Material Characterization Toolbox

Research Data Summary

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

Dataset name / ID	Description	New or reuse	Digital or Physical data	Data Type	File format	Data volume	Physical volume
		Indicate: N(ew data) or E(xisting data)	Indicate: **D**(igital) or **P**(hysical)	Indicate: **A**udiovisual **I**mages **S**ound **N**umerical **T**extual **M**odel **SO**ftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
ALAMEL	Original ALAMEL source code	E	D	SO	modern Fortran	<100GB	/
Code	The framework source code	N	D	SO	Various programming languages	<100GB	/
Feedback	Feedback from companies cooperating with framework development	E	D	T	Plain text	<1GB	/
Simulation results	Results from simulations	N	D	N	Text	<2 GB	/

If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type:

KU Leuven GitLab (https://gitlab.kuleuven.be/comp-mater-sci/TWRMTMProject).

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, refer to specific datasets or data types when appropriate and provide the relevant ethical approval number.

- No

We will ask users to provide feedback specifically on the software, but don't consider this as as "human subject data" because participants will speak for the company/research institution that they represent, not for themselves.

Will you process personal data? If so, please refer to specific datasets or data types when appropriate and provide the KU Leuven or UZ Leuven privacy register number (G or S number).

- No

Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, …)? If so,

please comment per dataset or data type where appropriate.

- Yes

The developed software has the potential for use by companies.

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material or Data transfer agreements, Research collaboration agreements)? If so, please explain in the comment section to what data they relate and what restrictions are in place.

- No

Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use? If so, please explain in the comment section to what data they relate and which restrictions will be asserted.

- No

Documentation and Metadata

Clearly describe what approach will be followed to capture the accompanying information necessary to keep data understandable and usable, for yourself and others, now and in the future (e.g. in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, codebook.tsv etc. where this information is recorded).

All code will be maintained in KU Leuven GitLab. The standard Git conventions are followed. The existing ALAMEL code already contains some documention based on DoxyGen, which will be expanded and structurized during the project.
New code will also be documented directly in the source files, using the conventions appropriate for the programming language used. Additionally, a user manual in PDF and/or JuPyteR notebook form will be provided for new users.
Company feedback will be stored as plain text within on KU Leuven computers for internal reference during development. As soon as the feedback has been integrated into the code or has otherwise becomes irrelevant, it will be deleted.

Will a metadata standard be used to make it easier to find and reuse the data?
If so, please specify which metadata standard will be used.

If not, please specify which metadata will be created to make the data easier to find and reuse.

- Yes

DoxyGen
JuPyteR notebooks

Data Storage & Back-up during the Research Project

Where will the data be stored?

- Other (specify below)

KU Leuven GitLab

How will the data be backed up?

- Personal back-ups I make (specify below)
- Standard back-up provided by KU Leuven ICTS for my storage solution

For locally stored feedback from companies:
[Unit]
Description=Daily backup to CS file server
[Timer]
OnCalendar=*-*-* 12:15:00
[Service]
User=stijn
ExecStart=/usr/bin/rsync --progress -a --exclude .* --include .vimrc --exclude Downloads --exclude intel --exclude docker /home/stijn/
stijns@simpson.cs.kuleuven.be:backup/

Is there currently sufficient storage & backup capacity during the project?

If no or insufficient storage or backup capacities are available, explain how this will be taken care of.

- Yes

How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?

KU Leuven GitLab uses the standard KU Leuven central login.
KU Leuven computers used during the project are protected using a password.

What are the expected costs for data storage and backup during the research project? How will these costs be covered?

No special costs are required.

Data Preservation after the end of the Research Project

Which data will be retained for 10 years (or longer, in agreement with other retention policies that are applicable) after the end of the project?

In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).

- All data will be preserved for 10 years according to KU Leuven RDM policy

Where will these data be archived (stored and curated for the long-term)?

- Other (specify below)

Code will be stored long-term on the KU Leuven GitLab server.
Company feedback stored on KU Leuven computers is backed up to the CS file servers.

What are the expected costs for data preservation during the expected retention period? How will these costs be covered?

No special costs are incurred.

Data Sharing and Reuse

Will the data (or part of the data) be made available for reuse after/during the project?
Please explain per dataset or data type which data will be made available.

- No (closed access)
- Yes, as open data
- Yes, as restricted data (upon approval, or institutional access only)

As stated in the project proposal, we aim to provide the computational core of ALAMEL as open-source software.

If access is restricted, please specify who will be able to access the data and under what conditions.

The paid features of the proposed framework will not be accessible by end users. Instead, they use the application through the internet. Feedback from companies will obviously not be available to future users as it is not relevant to them.

Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?

Please explain per dataset or data type where appropriate.

- No

Where will the data be made available?

If already known, please provide a repository per dataset or data type.

- Other data repository (specify below)

GitHub

When will the data be made available?

- Other (specify below)

The part of the code we plan to make open-source will be made available as soon as we competed modernizing and documenting it.

Which data usage licenses are you going to provide?

If none, please explain why.

- Other (specify below)
- GNU GPL-3.0 (code)

To use the framework, we will require companies to purchase a license from KU Leuven. The details of this license are to be determined in

collaboration with LRD.

Do you intend to add a persistent identifier (PID) to your dataset(s), e.g. a DOI or accession number? If already available, please provide it here.

- No

What are the expected costs for data sharing? How will these costs be covered?

No extra costs will occur for sharing data as existing KU Leuven infrastructure will be used.

Responsibilities

Who will manage data documentation and metadata during the research project?

Stijn Schildermans

Who will manage data storage and backup during the research project?

Stijn Schildermans

Who will manage data preservation and sharing?

Stijn Schildermans

Who will update and implement this DMP?

Martin Diehl
Stijn Schildermans

Created using DMPonline.be. Last modified 06 March 2024

6 of 6