CELSA/23/023

A Data Management Plan created using DMPonline.be

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Project abstract:

Novel materials with improved properties are critically needed for the transition into a sustainable circular economy. The challenging task of developing such materials requires reliable predictive simulation tools to complement time and cost expensive experimental characterization. With High-Performance Solvers for Multi-Physics Materials Simulations (HyPerMatSim) we propose to improve numerical robustness and performance of DAMASK1, an established open source crystal plasticity and multi-physics simulation toolbox, by developing and implementing novel numerical solvers based on the fast Fourier transform (FFT). The combination of state of the art numerical methods for solving partial differential equations with millions of unknowns in a memory- and resource-efficient way with physics-based constitutive models for plasticity, fracture, temperature, and chemical processes enables predicting the behavior of complex materials.

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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	
1	source code	n	d	other	*.f90	< 1GB	n/a

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:

code will be based on DAMASK (https://damask.mpie.de)

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

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.

- No

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.

- Yes

yes, code is licensed according to AGPL v3

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 developed using Git and GitLab

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.

- No

Data Storage & Back-up during the Research Project

Where will the data be stored?

gitlab.kuleuven.be

How will the data be backed up?

- Standard back-up provided by KU Leuven ICTS for my storage solution

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?

version control

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

0.0 EUR

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)

gitlab.kuleuven.be

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

standard research infrastructure or using public host such as github

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.

- Yes, as open data

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

Question not answered.

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)

gitlab.kuleuven.be

When will the data be made available?

per default

Which data usage licenses are you going to provide?

If none, please explain why.

- Other (specify below)

APGLv3

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?

0.0 EUR

Responsibilities

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

Martin Diehl and researcher (to be hired)

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

Martin Diehl and researcher (to be hired)

Who will manage data preservation and sharing?

Martin Diehl and researcher (to be hired)

Who will update and implement this DMP?

Question not answered.