
Plan Overview

A Data Management Plan created using DMPonline

Title: Probabilistic discovery of new microstructure-property relationships in advanced alloys

Creator: Joao Quinta da Fonseca

Principal Investigator: Joao Quinta da Fonseca

Data Manager: Joao Quinta da Fonseca

Affiliation: University of Manchester

Template: EPSRC Data Management Plan

ORCID iD: 0000-0001-6063-8135

Project abstract:

Our aim is to revolutionize metallurgical practice, by enabling data-centred exploration and discovery of deformation mechanisms in advanced alloys by developing a novel, invertible, probabilistic modelling framework. Recently, there has been an explosion of the applications of machine learning methods to develop predictive models in material science. Yet often such predictive models are scientifically unsatisfactory since they are unidentifiable. That is, it is not possible, or at best extremely difficult, to identify the mechanism or physics which contribute to the observed response. This proposal flips the traditional machine learning approaches on their head, by building so called invertible neural networks for material discovery. Instead of building predictive models, maps from inputs to outputs, we will use high fidelity state-of-the-art-computational models and large, dense time-resolved data sets to train a specific probabilistic neural network architecture which is invertible. The resulting, probabilistic framework developed will be able to identify (with associated uncertainty) the inputs which directly lead to a given output. Therefore, the outputs from this proposal will develop a novel computational tool for the discovery of new microstructure-property relationships in advanced alloys

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Probabilistic discovery of new microstructure-property relationships in advanced alloys

UoM Project Details

Proposal title

Probabilistic discovery of new microstructure-property relationships in advanced alloys

Is the project already funded?

- No

Will the project make use of data (please select all that apply)?

- Re-use existing data (please list below)
- Acquire new data

Where will the data be stored and backed-up during the project lifetime?

- Other repository or storage system (please provide details below)

Data will be stored on [Zenodo](#)

How much data storage will you require?

- > 8TB (please provide details)

Synchrotron data in particular will require a lot of space. We estimate 10-20 TB over the 5 years.

Data Collection

What data will you collect or create?

Experimental (physical data):

- text files
- binary files
- images

We will use standard, open file formats when possible.

How will the data be collected or created?

Very varied techniques.

Documentation and Metadata

What documentation and metadata will accompany the data?

We are going to use at the beginning a simple set of metadata which will be the bare minimum needed by Zenodo data repository. We are going also to define a set of metadata specific to the project but following as much as possible metadata standard with eventually additional informations needed for the specificities of the project.

Ethics and Legal Compliance

How will you manage any ethical issues?

There not ethical issue for this project.

How will you manage copyright and Intellectual Property Rights (IPR) issues?

Individual agreements with collaborators.

Storage and Backup

How will the data be stored and backed up during the research?

During data processing analysis the data will be stored in the Manchester RDS.

Once completed, data and analysis will be uploaded after creation and a first curation to be sure that they are consistent and with the proper metadata to the data repository (Zenodo). The upload will be eased by the usage of a dedicated software which will verify the presence of the needed metadata.

How will you manage access and security?

Most of the data will be placed under open data license. For the one which will need to have an embargo or to be closed, Zenodo is providing the necessary tool to allow that. Sharing can be done specifically by asking the data creators through Zenodo.

Security is provided by Zenodo.

Selection and Preservation

Which data are of long-term value and should be retained, shared, and/or preserved?

Most of the data created by the project will be kept for future usage or to be used by other members of the collaboration. Zenodo is providing the space which allows that conservation.

What is the long-term preservation plan for the dataset?

Zenodo via the community facility

Data Sharing

How will you share the data?

Data will be shared between the members of the project as soon as they are produced. At the end of the project most of the data under embargo will be shared under an open data license. Some data, coming from industrial partners, could be kept closed but with a contact person if needed.

Are any restrictions on data sharing required?

For some projects with substantial industrial funding, yes.

Responsibilities and Resources

Who will be responsible for data management?

Joao Fonseca and Project RSE

What resources will you require to deliver your plan?

RSE time and intermediate data storage (RDS).