Plan Overview

A Data Management Plan created using DMPonline

Title: Modelling tools for complex systems: advancing the capability of many body dissipative particle dynamics

Creator: Andrew Masters

Principal Investigator: Andrew Masters

Data Manager: Andrew Masters

Affiliation: University of Manchester

Template: EPSRC Data Management Plan Customised By: University of Manchester

ORCID iD: 0000-0003-3998-1769

Project abstract:

To develop new computational tools to be incorporated into Many Body dissipative particle dynamics methodologies so as to better control both equilibrium and dynamical properties.

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Copyright information:

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Modelling tools for complex systems: advancing the capability of many body dissipative particle dynamics

Manchester Data Management Outline

1. Is this project already funded?

- No

2. If you will be applying for funding from multiple sources who else will you be applying to?

- Not applicable

3. Is The University of Manchester the lead institution for this project?

- Yes – leading a collaboration

4. What data will you use in this project (please select all that apply)?

- Acquire new data

The project involves the creation of new algorithms for which pre-exising data are not required.

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

- University of Manchester Research Data Storage Service (Isilon)

6. If you will be using Research Data Storage, how much storage will you require?

- < 1 TB

7. If you have a contractual agreement with a 3rd party data provider will any of the data associated with this project be sourced from, processed or stored outside of the institutions and groups stated on your agreement?

- Not applicable

8. How long do you intend to keep your data for after the end of your project (in years)?

- < 5 years

Questions about personal information

Personal information or personal data, the two terms are often used interchangeably, relates to identifiable living individuals. Special category personal data is more sensitive information such as medical records, ethnic background, religious beliefs, political opinions, sexual orientation and criminal convictions or offences information. If you are not using personal data then you can skip the rest of this section.

Please note that in line with data protection law (the General Data Protection Regulation and Data Protection Act 2018), personal information should only be stored in an identifiable form for as long as is necessary for the project; it should be pseudonymised (partially de-identified) and/or anonymised (completely de—identified) as soon as practically possible. You must obtain the appropriate ethical approval in order to use identifiable personal data.

- No sensitive or personal data

10. Please provide details of how you plan to store, protect and ensure confidentiality of the participants' information as stated in the question above

We will have no such information.

11. If you are storing personal information will you need to keep it beyond the end of the project?

- Not applicable

12. Sharing person identifiable information can present risks to participants' privacy, researchers and the institution. Will the participants' information (personal and/or sensitive) be shared with or accessed by anyone outside of the University of Manchester? This includes using 3rd party service providers such as cloud storage providers or survey

platforms.

- No

13. If you will be sharing personal information outside of the University of Manchester will the individual or organisation you are sharing with be outside the EEA?

- Not applicable

14. Are you planning to use the personal information for future purposes such as research?

- No

15. Who will act as the data custodian or information asset owner for this study?

Andrew John Masters

16. Please provide the date on which this plan was last reviewed (dd/mm/yyyy).

Data Collection

What data will you collect or create?

Numerical data, such as molecular co-ordinates generated by a simulation.

How will the data be collected or created?

It will be created by a dissipative particle simulation code. The data will be lists of numbers, stored typically in a binary format. The volume of data to be stored will be typically 10 - 100 MByte.

Documentation and Metadata

What documentation and metadata will accompany the data?

All necessy documentation as to the use of our algorithms will be published online, along with useful metadata to help other potential users. Access will be free. All publications will contain required meta-data and documentation in supplementary documentation.

Ethics and Legal Compliance

How will you manage any ethical issues?

No ethical issues are anticipated, but if they arise, we will seek advice from the University of Manchester.

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

This will be managed via University of Manchester institutions (e.g. UMIP).

Storage and Backup

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

On hard-discs on the University of Manchester's Computer Shared Facility.

How will you manage access and security?

There is no restricted access to our data. Storage of data and access to it will be manged by he investigators, taking advice from the University of Manchester's Research IT team.

Selection and Preservation

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

We anticipate that we will generate no data of long-term value. The project is about methodologies. In case we do need to retain any data long-term, we will seek advice from Manchester's Research IT.

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

Again we foresee no need for long-term preservation of data. In the unlikely event this is needed, we will agin make use of the University of Manchester's long-term storage facilities.

Data Sharing

How will you share the data?

Data will be made freely available on request. Our website and supplementary information provided in our papers will also give free access to data.All our publications will be free access. Data will also be stored on the FactSage thermochemical data base.

Are any restrictions on data sharing required?

No

Responsibilities and Resources

Who will be responsible for data management?

Andrew John Masters

What resources will you require to deliver your plan?

Only the data management resources already provided by the University of Manchester.