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D 3.1 FAIR Data Management Plan

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CO	Confidential, only for members of the consortium (including the Commission Services)	
CI	Classified, as referred to in Commission Decision 2001/844/EC	

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3 Definition and Acronyms

Acronyms	Definitions
CDI	Collaborative Data Infrastructure
CoE	Centre of Excellence
DICOM	Digital Imaging and Communications in Medicine (DICOM) is a standard for handling, storing, printing, and transmitting information in medical imaging
DMP	Data Management Plan
DoA	Description of the Action
EUDAT CDI	An EU funded Collaborative Data Infrastructure
FAIR data	Findable, Accessible, Interoperable & Reusable Data
HDPA	High performance data analytics
HPC	High Performance Computing
IPR	Intellectual Property Rights
MIBBI	Minimum Information for Biological and Biomedical Investigations
OAI-PMH	The Open Archives Initiative Protocol for Metadata Harvesting
OpenAIRE	The Open access infrastructure for research in Europe
PDB	Protein Data Bank
VECMA	Verified Exascale Computing for Multiscale Applications (EU Project)
VVUQ	Verification, Validation, and Uncertainty Quantification

4   Introduction

This deliverable responds to the standard questions that must be answered to produce an initial H2020 data management plan (DMP). The DMP presented in the remainder of this document was produced using the DMPOnline tool available at: https://dmponline.dcc.ac.uk/.

It is based on the DMP of the predecessor Centre of Excellence (CoE), CompBioMed.

5   Data Summary

Provide a summary of the data addressing the following issues:

- **State the purpose of the data collection/generation**
- **Explain the relation to the objectives of the project**
- **Specify the types and formats of data generated/collected**
- **Specify if existing data is being re-used (if any)**
- **Specify the origin of the data**
- **State the expected size of the data (if known)**
- **Outline the data utility: to whom will it be useful**

CompBioMed2 is the second phase of the Computational Biomedicine Centre of Excellence (CoE), CompBioMed is an outward facing CoE comprising members from academia, industry and the healthcare sector. Its core purpose is to facilitate the uptake and exploitation of HPC-based Computational Biomedicine simulation approaches to a greater number of therapeutic areas.

Understanding the complex outputs of such simulations requires the convergence of High Performance Computing (HPC) and high-performance data analytics (HPDA). CompBioMed2 seeks to combine these approaches with the large, heterogeneous datasets from medical records and from the experimental laboratory to underpin clinical decision support systems. All data collected, used and generated by the project is done in support of this objective.

The project's three core research strands focus on the areas of cardiovascular, musculoskeletal and molecular-based modelling. Each of these scientific communities and associated software packages employ different data formats. Major types of data comprise:
- **Imaging data** which stem mostly from clinical trials, experiments, or visualised results of the simulations. They may serve as initial data for data analytics and machine learning tasks. Typical file formats used for these data are JPG, PNG, DICOM, MP4, and MOV.
- **Other clinical and experimental data** which serve as reference for simulations. Here a broad variety of file formats are used from formatted/unformatted plain text, PDF and DOCX files, tabulated data formats like CSV and XLSX, as well as (raw) binary data.
- **Musculoskeletal data** which record the motion of joints, bones, muscles, etc. They are the key output of musculoskeletal simulations and use file formats such as C3D and XMDF.
- **Cardiovascular data** resulting from heart and blood flow simulations in the project are mostly recorded in HDF5 and VTK file formats.
- **Molecular-based modelling data**: Structures of complex biomolecules, assemblies thereof, smaller molecules and molecular dynamics trajectories serve as initial conditions or are output of simulations conducted in the project and may be targets of

HDPA approaches. Most frequently used file formats are PDB, PSF, XTC, TRR. A variety of tools are available that are able to read and convert these different formats.

ComBioMed2 is a large Centre of Excellence, comprising not just funded core partners, but also a growing network of associate partners who seek to participate in the Centre's activities and bring in their own data and data formats. Thus, the above list is long but by no means complete.

CompBioMed2 builds on the data stock of the predecessor CoE, CompBioMed, but it is not actively involved in assembling initial datasets. These are brought to the project by its partners, e.g. from the cardiovascular, molecularly-based and neuro-musculoskeletal exemplary research, tasks 2.1-2.3, and the "Analytics for in silico augmented clinical trials", task 3.6. The data originate from many different sources: Non-simulation data, used to build models generally, can originate from clinical data management systems or DICOM image stores or from biochemical structure databases such as Protein Data Bank (PDB; http://www.rcsb.org/pdb/). Simulation results are generated from computational models that are run on HPC resources around Europe.

The size of the data the project needs to store largely depends on the time frame and the level of postprocessing and/or compression applied. A sufficient volume of immediate storage for input and output data is typically provided by the HPC centre, where the simulations are conducted. Long-term storage or archive systems are usually based on tape media, which are cheaper compared to disk storages and therefore have less limitations on the size of data they store. The tape storage however, imposes a latency in retrieving the data and therefore limits its accessibility. We estimate the total size of raw data that will be generated by the project during its lifetime to exceed 4 PB, but much less may be required to be stored by CompBioMed2.

The data managed and produced within the project is of immediate use to medics, clinicians and researchers, the key areas of the CompBioMed2 CoE, and in the intermediate term to industrial researchers and drug/medical device manufacturers and ultimately to patients. The data produced by the project is typically generated by software and workflows developed in the project, and therefore correspond to specific versions of that software. Task 3.4 of the CompBioMed2 project is dedicated to data curation. It will promote the reuse of data, through the application of annotation and metadata, which will make the data more amenable to analytics technologies and make data more easily found and reused by other researchers.

6 FAIR Data

We as CompBioMed2 CoE strictly adhere to EU's open science policy, namely https://ec.europa.eu/info/research-and-innovation/strategy/goals-research-and-innovation-policy/open-science_en. To measure the project performance with respect to the FAIR principles, we introduced the KPI "Number of data sets published openly with FAIR principles".

In our recent bi-annual data survey (Dec. 2020) we also monitored the data produced and published by the project. Most partners (> 90%) indicated that they did or intend to publish raw or pre-processed data that relate to published work after a suitable embargo period. This covers metadata possibly combined with data online for download or made available upon request. Most partners (>50%) publish their data on the platform of the journal or on the platform of their institution/university, while other repositories such as Zenodo and the B2SHARE service from the EUDAT CDI were much less used (<10 %).

CompBioMed2 core partners are required to adhere to FAIR (Findable, Accessible, Interoperable, and Re-usable) principles for all data that is generated within simulations and the analysis of existing data. To ensure that all partners have the necessary knowledge and apply open science research routines and practices, Work Package 3 offers support and training on FAIR principles. After each biannual data survey WP3 proactively contacts researchers who have indicated to publish their data on the platform of the journal and guide them in publishing their data sets via B2SHARE. Online trainings on FAIR data publishing are offered (see e.g. https://www.compbiomed.eu/compbiomed-webinar-9/) throughout the project. For immediate contact with the data publishing support, the recently set up "Data Publication Channel" within the CompBioMed2 slack project "In Silico World" can be contacted. The channel is regularly monitored by WP3 members. They offer help on various data publication topics such as available platforms, annotation schemes, etc. With respect to the associate partners, CompBioMed does not have control over how this data is published and made available. Nevertheless, CompBioMed encourages partners to follow the FAIR principles and offers help. These efforts are promoted by task 3.4 "Data Curation" of the project, which offers support to the core and associate partners of the CompBioMed2 CoE.

For documentation, the relevant mandatory metadata of data published in the CompBioMed community (DOI (Digital Object Identifier), repository link (or non-repository link), title, is dataset accessible (Y/N), is dataset reusable (Y/N)) and optionally the DOI linked publication will be provided on the Commission Portal.

6.1   Findable Data

Making data findable, including provisions for metadata:

- **Outline the discoverability of data (metadata provision)**
- **Outline the identifiability of data and refer to standard identification mechanism. Do you make use of persistent and unique identifiers such as Digital Object Identifiers?**
- **Outline naming conventions used**
- **Outline the approach towards search keyword**
- **Outline the approach for clear versioning**
- **Specify standards for metadata creation (if any). If there are no standards in your discipline describe what metadata will be created and how**

For data generated by research conducted within the project, we mandate that the final results of any simulation can be made discoverable. UCL has been and is a participant in the EUDAT and EUDAT2020 projects, and has joined the EUDAT Collaborative Data Infrastructure (CDI) among other CompBioMed2 partners, such as BSC, EPCC, and SURF. EUDAT CDI operates the important platforms B2DROP and B2SHARE to upload, share and publish data, as well as B2FIND, which provides a search engine to find stored metadata. We therefore leverage the best practice and services which EUDAT provides to make data discoverable.

The EUDAT Consortium follows the OpenAIRE guidelines for Data Archives[1] by mandating standard minimal metadata and publication of metadata using the OAI-PMH protocol. We have already added CompBioMed as a community to the B2SHARE repository (please see https://b2share.eudat.eu/communities/CompBioMed) in which data can be published and searched later based on the community. For now, we are using the generic metadata schema

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[1] https://guidelines.openaire.eu

which is based on the Dublin Core Schema. Ideally, we aim to have a community-specific metadata schema defined and implemented in B2SHARE so that the CompBioMed2 researchers can publish their data with community-specific metadata.

Data that is being published in B2SHARE is harvested by B2FIND, which is a web metadata portal allowing researchers to easily find and access metadata on scientific data, and redirect the users to the origin of the data. In addition, data are documented with a content- or discipline-specific metadata record. The data generated by the project arise from a number of different interrelated fields, therefore not a single metadata standard applies to all the cases, but we work with data generators to identify suitable standards from the Research Data Alliance Metadata Standards Directory, which includes PDBx/mmCIF and MIBBI.

All the data that we publish via the EUDAT B2SHARE data repository service will be assigned a persistent identifier through the Handle system. This unique dataset reference can be used in data citations and to enhance discoverability. EUDAT B2SHARE provides an automatic versioning with ascending numbers and time indices that allows a clear identification of the dataset version.

This allows us to exploit the EUDAT B2FIND catalogue to make data keyword searchable, either via the B2FIND web interface or the application programming interfaces OAI-PMH, JSON-API, CSW2.0 as outlined in http://b2find.eudat.eu/guidelines/harvesting.html.

We initiated collaborations with other EU initiatives and projects such as EOSC's DICE project and LEXIS. The DICE/CompBioMed2 collaboration aims to deploy their own dedicated B2SHARE instance at UCL with dedicated storage in the backend. This is pivotal as the community instance of the B2SHARE repository on https://eudat.eu/services/b2share only allows for a maximum record size of 20GB and a maximum file size of 10GB and is thus designed for the publication of comparably small data sets. It is worth noting that space in this repository is hosted on CompBioMed servers/data storage systems. The LEXIS/CompBioMed2 collaboration, by contrast, aims to build an advanced, geographically-distributed HPC infrastructure for Big Data analytics. Within both the cooperation and Task 3.3 "*Data Staging Systems*", the HPC centres LRZ, SURF, BSC and EPCC at UEDIN are federated based on B2SAFE and workflows involving data staging are conducted.

6.2   Accessibility

Making data openly accessible:

- **Specify which data will be made openly available? If some data is kept closed provide rationale for doing so**
- **Specify how the data will be made available**
- **Specify what methods or software tools are needed to access the data? Is documentation about the software needed to access the data included? Is it possible to include the relevant software (e.g. in open source code)?**
- **Specify where the data and associated metadata, documentation and code are deposited**
- **Specify how access will be provided in case there are any restrictions**

In general, all data that relates to published work and has been generated within CompBioMed2 will be made available after a suitable embargo period (as defined by the relevant journal). However, legal, ethical or IPR barriers may prohibit specific data to be published with

unrestricted access. Here, the CompBioMed2 project works with the data owners to identify whether the data can be made open after a period of embargo or if other measures can be applied to alleviate such restrictions. We make use of the features of EUDAT that allow depositors to choose to keep data private, password protected, or to apply embargo periods. It should be noted that metadata will always be openly available in B2SHARE, even though the data is chosen to be private.

The B2SHARE repository is a user-friendly, reliable and trustworthy way for researchers to store and share research data from diverse contexts. It guarantees long-term persistence of data and allows data, results or ideas to be shared worldwide. CompBioMed2 has implemented the dedicated task 3.2 "Data Storage System Deployment and Maintenance" for this purpose.

The metadata contain references to the software and version that were used to generate the data, which are generally CompBioMed2 modelling tools. A comprehensive list of these tools is featured on the CompBioMed2 project website at https://www.compbiomed.eu/services/software-hub/.

CompBioMed2 will also make use of the B2DROP service provided by EUDAT for sharing live data internally in the project. B2DROP is an online cloud storage tool to store and exchange data with collaborators and to keep data synchronized and up-to-date. This will ease the transition to making data openly available in future, as B2DROP is linked to the B2SHARE data repository. CompBioMed2 will take advantage of the free storage space provided for research data within the B2DROP framework.

6.3   Interoperability

Making data interoperable:

- **Assess the interoperability of your data. Specify what data and metadata vocabularies, standards or methodologies you will follow to facilitate interoperability.**
- **Specify whether you will be using standard vocabulary for all data types present in your data set, to allow inter-disciplinary interoperability? If not, will you provide mapping to more commonly used ontologies?**

In general, data used and created by the project is stored in standard formats such as DICOM and PDB. Data will be annotated with the metadata standards mandated by EUDAT when it is deposited, along with appropriate standard from the Research Data Alliance Metadata Standards Directory.

Because of the vast array of data types arising from within the CompBioMed2 CoE, it is impossible to define a single interoperability standard, and the project does not have sufficient resources available to enforce ontological annotation. However, task 3.4 "Data Curation" will supply guidance for researchers to annotate their data using popular ontologies.

6.4   Reuse

Increase data re-use (through clarifying licenses):

- **Specify how the data will be licenced to permit the widest reuse possible**
- **Specify when the data will be made available for re-use. If applicable, specify why and for what period a data embargo is needed**
- **Specify whether the data produced and/or used in the project is useable by third parties, in particular after the end of the project? If the re-use of some data is restricted, explain why. Describe data quality assurance processes**
- **Specify the length of time for which the data will remain re-usable**

We expect core project partners to deposit their data openly using a Creative Commons version 4.0 licence or equivalent. Our IP (Intellectual Property) restrictions applying to, for example, industrial partners, state that all data are made publicly/openly available at the conclusion of the relevant tasks of CompBioMed2. Reasons for exceptions must be explicitly stated. In the course of the project we regularly inquire with the individual tasks, which data have been published and offer help with metadata annotation. We also encourage our associate partners to adopt similar policies, and promote these policies at CompBioMed2 training events.

Data reuse is also promoted within the project, when data generated by simulations is analysed with deep learning and machine learning techniques by different tasks across work packages. Similarly, these data may be of interest and could be analysed by related CoEs focusing on computational biomolecular research such as BioExcel2 (https://bioexcel.eu/).

The EUDAT B2SHARE service allows data to be shared openly or kept private. Regardless of the privacy of the deposited data, metadata records (such as, e.g., Title, PID, Publication Date, Contact Email) submitted as part of a data deposit are made freely available for harvesting via OAI-PMH protocols. Accessible data is made available directly to users of EUDAT CDI services through graphical user interfaces and application programming interfaces. We make published data available for third-party use as long as the EUDAT B2DROP platform is able to host it. If relevant data exceeds this limit, we will explore other possibilities within task 3.2 "Data Storage System Deployment and Maintenance". The use of open standard formats, metadata annotation and workflow documentation (on the CompBioMed2 software portal) helps to ensure data quality with respect to documentation and completeness. For the reliability of the data generated by simulations, CompBioMed2 closely collaborates with the VECMA project to provide VVUQ for the methods used. Here, VVUQ stand for **V**alidating that the model underlying the simulation is sufficiently accurate, **V**erifying that the model is implemented correctly and **Q**uantifying the statistical **U**ncertainty to e.g. the finite time span of the simulation or the limited resolution of the model. All these points are fundamental for the quality and reliability of the data.

7   Allocation of Resources

Explain the allocation of resources, addressing the following issues:

- **Clearly identify responsibilities for data management in your project**
- **Describe costs and potential value of long-term preservation**

As outlined in section 6 we largely build on the services provided by the EUDAT project to make our data FAIR compliant. EUDAT CDI services generally come for free and we get the required technical support for deploying and maintaining these services via collaborations with EOSC and DICE projects. Furthermore, the CompBioMed2 partners UCL, BSC, EPCC, and SURF are members of EUDAT, so we don't anticipate incurring any further costs to use these services.

Project data management is primarily the responsibility of individuals leading tasks that generate data within the project. With task 3.4, CompBioMed2 has allocated dedicated PMs to support core and project partners enforcing FAIR principles.

We leverage EUDAT B2SHARE for the long-term preservation of data. In addition, SURF is a partner in the EUDAT consortium, leading the work package that develops and maintains the B2SAFE EUDAT service. Furthermore, the HPC centres, which provide compute time allocations for CompBioMed2 projects, offer tape archives for long term storage of large data sets; such providers are SURF, EPCC, BSC, and LRZ. Currently, no additional costs arise for CompBioMed2.

8   Data Security

Address data recovery as well as secure storage and transfer of sensitive data

Internally, within the project, file-based data will be shared using the EUDAT B2DROP and B2STAGE services for secure transfer. Other types of data, such as DICOM image data, will be stored at data centres of the core partners such as UCL and UOXF, making use of the access control and secure transfer features provided by the service in question, and taking advantage of UCL's central data centre management policies. Support for the project partners is implemented in task 3.3 "Data Staging Systems" of CompBioMed2.

Data shared and published via the EUDAT CDI will be stored at one or more partner sites, according to applicable service level agreements and policies. Backup of data is performed at two levels using the B2SAFE service: multiple replicas of data are stored at different sites (i.e. geographically and administratively different); and data may additionally be backed up at an individual site. Responsibility for the storage and backup at any individual site lies with the designated site manager.

All EUDAT CDI core sites are large, national or regional data and computing centres and operate according to good IT governance and information security principles. Some sites are accredited through the ISO 27001 information security process and/or have certifications of trustworthiness such as the Data Seal of Approval, while others are working actively towards it.

For more information and to show that data safety is an important concern of CompBioMed2, we created an overview page on https://www.compbiomed.eu/data-security-policy/ containing the data security policies of the four HPC centres within CompBioMed2, namely BSC, EPCC, LRZ and SURF.

9   Ethical Aspects

To be covered in the context of the ethics review, ethics section of "Description of the Action" (DoA) and ethics deliverables. Include references and related technical aspects if not covered by the former

CompBioMed2 as a CoE does not actively collect data from individuals, and simulation scenarios are largely based on publicly obtainable/consented data that has been provided to project partners (core and associate, as well as via other collaborations).

Regarding data governance, CompBioMed2 is not intended as a facility for the routine processing of live, identifiable clinical data; it operates in the research domain, and all data introduced by users will be required by the CompBioMed2 conditions of use to be pre-processed to render it non-personal, and so to be excluded from consideration under current and anticipated future research governance regulations. CompBioMed2 will, however, act as a Data Controller for the information relating to the registration and access control of its users, and such data will be handled in full accordance with appropriate pan-European legislation.

Regarding data ethics, the CompBioMed2 framework is designed to support independent users in their access to large-scale computational facilities. It enables users to work with models, applications and data for which they are responsible, in the pursuit of their own research goals. Users sharing data must do so under the terms granted by the data's original ethical sanction, and again users will be required by the CompBioMed2 conditions of use to reach documented agreement that the terms of ethical sanction have been met. It is the case, however, that ultimately CompBioMed2 cannot take responsibility for the provenance or ethical compliance of data shared through its infrastructure, nor can it take account of the diverse legislation and the variable interpretation of European directives that may occur in the various Member States. Some tasks within CompBioMed2 access and analyse clinical data. Here, the corresponding CompBioMed2 task should be considered a *Data Manager*, which is delegated by the *Data Provider* (typically a hospital) to handle clinical data, for which the data provider has received from the *Data Owner* (the patient) the necessary permission to allow the treatment to be accessed by one or more *Data Consumers* (typically modelling experts) in order to fulfil a certain treatment scope. In order to be legally compliant, clinical data require two things: the permission to treat from the data owner (the patient), and an adequate protection of confidentiality. This in turn implies:

1. CompBioMed2 can handle only clinical data for which access has been granted. All users are fully responsible for ensuring that the necessary permission has been acquired. CompBioMed2 will assist not-for-profit users such as research hospitals or universities by providing them with informed consent templates (written by an expert) that provide the type of permission necessary for a given treatment using the CoE's tools and services.

2. Full anonymisation: when the processing of the data does not require the distinguishing of one individual patient from another, if necessary CompBioMed2 will provide a server, to be installed behind the hospital firewall, that will automate the replication of selected data to CompBioMed2 storage, while providing automated semantic annotation according to popular ontologies, and irreversible anonymisation according to agreed rules. This server will be managed by the hospital staff.

3. Pseudo-anonymisation via a trusted third party: if the identity of the patient cannot be entirely removed (for example, for personalised clinical treatment), the type of infrastructure is the same as (2) above but this time the data are annotated with a PatientID that remains within the safety of the hospital secure network, associated with the patient's actual identity.

Any further ethical and corresponding legal issues regarding handling of sensitive data that may arise during the project will be addressed by the "Ethics Panel" implemented within the task 3.7 "Ethics" of work package 3 "Data Management and Analytics."

10 Other

Refer to other national/funder/sectorial/departmental procedures for data management that you are using (if any)
N/A