

CHAMP is an HPC Access and Metadata Portal

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Software

- Review 🗗
- Repository 🗗
- Archive ♂

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Summary

CHAMP (CHAMP is an HPC Access and Metadata Portal) provides an easy to use workflow for FAIR data generation and publication using high performance computing (HPC) resources. It provides a web based interface allowing submission of HPC workloads and subsequent one-click publication of the results to data repositories such as Zenodo. Depositions support rich metadata to repositories that include a full implemention of the Subject property of the DataCite metadata schema (DataCite Metadata Working Group, 2021).

Users submit jobs simply by choosing from pre-configured software and computing resource specifications:

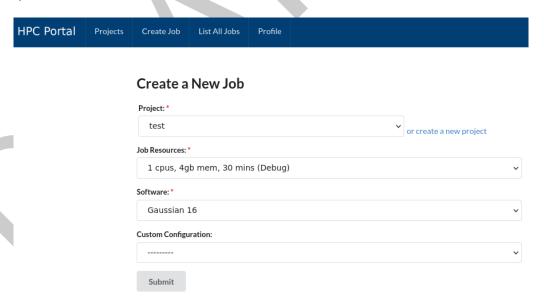


Figure 1: The form for the initial step in job creation

The user is then asked to upload the required input files for their chosen software and may optionally provide a job description:

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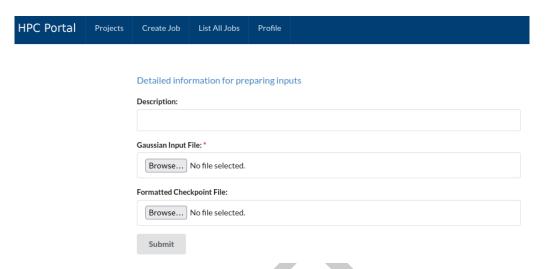


Figure 2: The form for the file upload step in job creation

- The status of jobs is available via a dedicated view. Publication to data repositories is also possible once the job has completed, with the reserved persistent identifier (a DOI) shown
- 19 associated with the job.

Job Number ♥	Software	Description	Resources	Status	Runtime	Submission time	Project	Directory	Repository	
0000004	Gaussian 16	an example Gaussian job	1 cpus, 4gb mem, 30 mins (Debug)	Completed	0:00:15	24/08/2021 8:57 p.m.	test	Open Download	10.5281/zenodo.5510302	Delete
00000003	Gaussian 16	-	1 cpus, 4gb mem, 30 mins (Debug)	Completed	Unknown	24/08/2021 8:56 p.m.	-	Open Download	Publish	Delete
0000001	Gaussian 16	-	GPU, 12hrs	Completed	0:00:15	11/08/2021 2:14 p.m.	-	Open Download	Publish	Delete

Figure 3: Summary table of jobs run using the portal

- ²⁰ CHAMP makes use of the Open OnDemand (Hudak et al., 2018) framework. This allows
- 21 CHAMP to be portable across different HPC systems and to integrate flexibly with institutional
- infrastructure (e.g. authentication mechanisms).
- 23 CHAMP represents over 15 years of experimentation in HPC portal design (Harvey et al.,
- 24 2014). The recent 2.0 release is a ground up rewrite to facilitate its publication as an
- open-source package, to modernise the code base and to address isues of portability and
- 26 sustainability.

Statement of Need

- ²⁸ Access to HPC resources has traditionally been available almost exclusively via command line
- interfaces which can present a barrier to entry for new and occasional users. The web interface
- provided by CHAMP is simple and intuitive providing an ideal entry point for non-experts.
- Open OnDemand, the framework used by CHAMP, also provides a web based interface for
- HPC job submission. CHAMP differs by providing a higher level of abstraction that completely
- 133 removes the need to deal with shell scripts or scheduler directives. This trade-off makes
- 34 CHAMP much easier to use but introduces the restriction that only pre-configured software
- 35 and resource configurations are supported.



- The ability to publish job outputs to data repositories greatly simplifies the process of producing
- metadata-enabled FAIR datasets. The relevant files to upload and various rich metadata items
- 38 are collected using workflows based on the selected software.

39 Implementation and Features

- 40 CHAMP is written as a Passenger App within the Open OnDemand (OOD) framework. It
- 41 must therefore be deployed within a local OOD instance. Use of OOD provides numerous
- 42 advantages such as portability, a strong security model and an active community of users.
- This allows the CHAMP code base to be quite minimal with mechanisms for authenticaton
- 44 and system scheduler interaction provided by the parent framework. The per-user NGINX
- architecture of OOD ensures all relevant computational processes are run under individual
- user UIDs.
- ⁴⁷ CHAMP is written in Python (>=3.7) using Django (Django Software Foundation, 2019) and
- 48 supports extensive customisation via its main YAML configuration file. Administrators may
- 49 configure the relevant software packages and resource configurations for their local system.
- 50 There are no restrictions on the software or resource types that may be configured. Arbitrary
- workflows may be used to run software and to generate metadata. This allows flexibility to
- e.g. use a job restart file if uploaded by a user or vary metadata for publication depending on
- job inputs.
- 54 The workflow that CHAMP imposes for HPC usage also provides inherent reproducibility.
- Individual jobs are structured within separate directories with relevant input files and scripts
- 56 present. Jobs are recorded with metadata such as resources used and a free text description
- 57 and are organised into projects. Job history can be filtered and searched according to this
- metadata allowing the portal to act as a simple electronic lab notebook.
- 59 An integration with Zenodo is included in the code base. Additional data repositories that
- support interaction via API and OAuth2 authentication may be configured via a plugin mech-
- anism. This allows the development of custom integrations with institutional data repositories
- 62 where desired, in the case of Imperial College with an existing repository service (Harvey et
- al., 2017).

4 Acknowledgments

- $_{65}$ We acknowledge the extensive contributions of Dr Matthew Harvey for work on version 1 of
- 66 this software.

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