

CHAMP is an HPC Access and Metadata Portal

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Software

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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 implementation 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:

The screenshot shows the 'Create a New Job' form on the CHAMP portal. At the top is a navigation bar with links: HPC Portal, Projects, Create Job, List All Jobs, and Profile. The form itself has four main sections: 'Project' with a dropdown set to 'test' and a link 'or create a new project'; 'Job Resources' with a dropdown set to '1 cpus, 4gb mem, 30 mins (Debug)'; 'Software' with a dropdown set to 'Gaussian 16'; and 'Custom Configuration' with a dropdown showing '-----'. A 'Submit' button is located at the bottom of the form.

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 associated with the job.

Job Number ▼	Software	Description	Resources	Status	Runtime	Submission time	Project	Directory	Repository	
00000004	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
00000001	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

CHAMP makes use of the Open OnDemand (Hudak et al., 2018) framework. This allows CHAMP to be portable across different HPC systems and to integrate flexibly with institutional infrastructure (e.g. authentication mechanisms).

CHAMP represents over 15 years of experimentation in HPC portal design (Harvey et al., 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 issues of portability and sustainability.

Statement of Need

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 removes the need to deal with shell scripts or scheduler directives. This trade-off makes CHAMP much easier to use but introduces the restriction that only pre-configured software and resource configurations are supported.

36 The ability to publish job outputs to data repositories greatly simplifies the process of producing
37 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.
43 This allows the CHAMP code base to be quite minimal with mechanisms for authentication
44 and system scheduler interaction provided by the parent framework. The per-user NGINX
45 architecture of OOD ensures all relevant computational processes are run under individual
46 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
51 workflows may be used to run software and to generate metadata. This allows flexibility to
52 e.g. use a job restart file if uploaded by a user or vary metadata for publication depending on
53 job inputs.

54 The workflow that CHAMP imposes for HPC usage also provides inherent reproducibility.
55 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
58 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
60 support interaction via API and OAuth2 authentication may be configured via a plugin mech-
61 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
63 al., 2017).

64 Acknowledgments

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66 this software.

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