PAPER

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DataVault: a data storage infrastructure for the Einstein Toolkit

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Abstract

Data sharing is essential in the numerical simulations research. We introduce a data repository, DataVault, which is designed for data sharing, search and analysis. A comparative study of existing repositories is performed to analyze features that are critical to a data repository. We describe the architecture, workflow, and deployment of DataVault, and provide three use-case scenarios for different communities to facilitate the use and application of DataVault. Potential features are proposed and we outline the future development for these features.

Keywords: numerical relativity, data repository, Einstein Toolkit, simulation storage

(Some figures may appear in colour only in the online journal)

1. Introduction

Numerical computing is a fundamental part of modern scientific research, with computer codes and their resulting data sets becoming ever more complex and costly to produce, maintain and support. Collaborations between different research groups around code development and use

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are now commonplace. These collaborations can be closed or open depending on whether new members can easily join and contribute to data sets and computer codes. Whichever form the collaboration takes, a platform to easily store, share and analyze data generated by or consumed by the collaboration is critical to the success of these collaborations.

Outside the field of astrophysics, data repositories are already widely used in different disciplines. For example, the Protein Data Bank (PDB) [1] is a repository of information about the 3D structures of large biological molecules, which enables users to deposit, search for, download, visualize and analyze PDB data. Zenodo [2], as another examples is a generic data repository that supports a broad wide range of domains and disciplines.

This paper provides a case study of a new data platform, 'DataVault' [3, 4], built to support the Einstein Toolkit community [5]. The Einstein Toolkit is a community-driven open-source software platform of core computational tools to advance and support research in relativistic astrophysics and gravitational physics. The user base includes more than 300 scientists distributed across 200 research groups worldwide who use different software components of the Einstein Toolkit to model scenarios in relativistic astrophysics, including black holes, neutron stars, supernovae and gravitational waves. A more detailed discussion of compact objects and gravitational waves, as well as their numerical simulations, can be found in [6, 7]. A recent review of gravitational waves and development of LIGO can be found [8].

DataVault is designed around a number of motivating use cases that are also common in other fields of computational science:

- Fostering collaboration across a geographically dispersed and loosely organized group of collaborators with a semi-private repository, where any collaborator can upload data sets. Users are able to query to see if data is already available for a particular parameter choice and then retrieve and analyze the results.
- Sharing the data produced by a scientific (sub-)community through a centrally hosted data repository to a wider science community. As an example, the initial target group for DataVault is the interaction between the numerical relativity (NR) community and waveform modelling groups that relies on sharing of data sets produced in NR simulation which are used to calibrate semi-analytic waveform models.
- Providing data sets produced within the scientific community to a wider, non-scientist audience via a well-defined, easy-to-use interface. This enables citizen science efforts as showcased, for examples, in the Citizen Science [9] and Galaxy Zoo [10] projects that make data accessible to a larger user base, such as high-school students and students at non-PhD granting universities.

In order to address these usage cases, we have designed DataVault, a web-based, domain specific data storage facility that can be easily used and deployed by groups interested in sharing their data products. We are specifically targeting the NR waveform community which exemplifies all three usage cases outlined above.

For the Einstein Toolkit community, we design the DataVault repository to achieve multiple functionalities for different researchers. We provide a large set of waveforms spanning a so far unexplored region of parameter space for scientists involved in gravitational waveform (GW) modeling. Users have a full set of functions to help them better share their data and metadata associated with it. As an open-source collaboration, DataVault and Einstein Toolkit project team members include faculty, research staff, as well as students world wide. This international collaboration shapes DataVault to better match current research needs and be more adaptive to new research directions.

Key functionality in DataVault to facilitate efficient data sharing among scientists includes:

Table 1. Comparison of existing repositories.

Repository	DataVault	GT	RIT	SXS	CoRE	Zenodo	IDB	FRDR
Open source	Yes	No	No	Yes[a]	No	Yes	No	No
Domain specific	Yes	Yes	Yes	Yes	Yes	No	No	No
Download metadata	Yes	Yes[b]	Yes[c]	Yes[d]	No	No	No	No
PID	Custom	Custom	Custom	DOI	Custom	DOI	DOI	DOI
Metadata extraction	Yes	N/A	N/A	N/A	N/A	No	No	No
Numerical search	Yes	No	Yes	Yes	No	No	No	No
Add collaborators	Yes	N/A	N/A	N/A	N/A	No	No	Yes
Upload by external users	Yes	No	No	No	No	Yes	No	Yes

[a] uses Zenodo code
[b] single text file
[c] tar archive
[d] single json file

- Advanced metadata searching using knowledge of the type of metadata stored in DataVault allows for quick selection of data sets that users want to study further. Moreover, DataVault, as an open-source project, can be modified by users to match their needs, potentially contributing the functionality back to the public DataVault code.
- Public data accessibility is an important factor underpinning results in a publication and enabling further research based on prior work. DataVault enables users to publish data sets they used in publications, so any readers can download the data to verify and further analyze their results conveniently. Data citation and validation of data sets are important factors in promoting data sharing. To this end DataVault provides a unique identifier for each data set as well as for collections of multiple data sets. DataVault supports both upload-restricted installations where data sets can only be uploaded by a pre-approved set of collaborators as well as open installations that allow users to register and upload their own data.
- An easy-to-use, well-defined interface provides the non-scientific public with access to scientific data sets for outreach purposes. Data stored in DataVault is made discoverable and interested users without in-depth familiarity with the research groups can easily access the data.

Organization of this paper. This manuscript is organized as follows: section 2 reviews existing data repositories used in numerical astrophysics, section 3 introduces DataVault's framework, section 4 outlines future directions for DataVault and section 5 contains our main conclusions and summary.

2. Existing repositories

This section provides an non-exhaustive study, summarized in table 1, of existing data platforms that have been built by individual numerical research groups or collaborations [11–14]. In addition the study includes generic platforms, such as Zenodo [2] and the Illinois Data Bank [15]. The study aimed to identify the capabilities and functionalities available in 8 different repositories, comparing them using the following criteria.

Open source. Is the source code of the repository infrastructure available under an open source license? An open source licensed repository encourages customization based on specific needs, and facilitates the sustainability of the data repository when its maintenance passes to new developers.

Domain specific. Is the repository a generic data repository or domain-specific repository that targets a specific user community?

Persistent Identifier (PID). Does the repository provide a PID for each data set that can be used as a citation? Data will be retrieved long after it was uploaded initially, making a PID mandatory.

Metadata extraction. When a user uploads the data set, can the repository process the data set with custom operations, such as metadata extraction and grouping multiple data sets into a collection?

Numerical search. Does the repository provide numerical search functionality beyond basic textual search? Users should be able to search for numerical ranges in metadata.

Downloadable metadata. Is the full set of searchable metadata available for download and offline processing? Complex queries beyond the provided search facilities can be implemented by experienced users using the raw metadata to select only specific data sets for download.

Add collaborators. Does the repository support multiple people to enter metadata and upload files for a submission? In this way, research groups can invite collaborators to contribute to a data set.

Upload by external users. Does the repository allow external users to upload their data sets? External users are defined as researchers that are not in the collaboration which either hosts or develops the catalog.

2.1. Repositories in the numerical astrophysics community

Multiple groups active in the field of numerical astrophysics have made their simulation results available to the public. In particular for the NR community that is the initial target community of DataVault, the numerical injection analysis (NINJA) [16] and numerical relativity analytical relativity (NRAR) [17] projects brought together numerical relativists and GW modellers. They, for the first time, defined a common data format used by multiple groups and all existing repositories of NR waveforms use formats descended from those defined by NINJA and NRAR.

This section provides a short review of the existing repositories of GWs. All currently existing repositories are maintained by individual research groups or collaborations, employing relatively straightforward web-frontends to the data hosted. They typically provide functionality to find waveforms based on parameters describing the simulation, as well as ways to download the full set of metadata describing the data in the repository.

For each repository we provide a short overview and summarize our findings in table 1. Since these are private repositories using, at least for some functionality, proprietary, non-disclosed code, we cannot report on the mechanism available to user to populate the database.

Georgia tech (GT) catalog of GW*s*. The GT Catalog of GWs [12, 18] is a domain-specific data catalog currently containing 452 distinct waveforms from binary black holes (BBH) simulations formerly maintained by the NR group at GT. The catalog is organized as a set of individual simulations in a 12-dimensional parameter space, including initial parameters of BBH and the resulting remnant black hole, along with a unique identifier and an internal name. Keyword search and sorting facilities are provided by proprietary JavaScript code on the website. The data for a given simulation is available in individual numerical relativity injection (NRI) [19] files stored on GitHub. Example scripts to read these files are provided via GitHub [20].

Rochester Institute of Technology (RIT) binary black hole simulations catalog. RIT NR group's catalog contains 777 BBH waveforms [14, 21, 22]. The catalog is organized as a set of individual simulations in a 20-dimensional parameter space, including initial parameters of BBH and remnant black hole along with a unique identifier and simulation parameters. Keyword and numerical range based search and sorting facilities are provided by proprietary JavaScript code on the website. The data for one or multiple simulation(s) can be downloaded. Simulation data is available as NRI format files stored at RIT. In addition metadata is provided in NRAR format files [17] files, a predecessor of the NRI format.

Simulating eXtreme Spacetimes (SXS) GW database at Cornell. The SXS GW database [11, 23] consists of 2018 black hole and neutron star merger simulations. The catalog if organized as a set of individual simulations in a 90-dimensional parameter space, including initial parameters of BBH or neutron stars and remnant black hole or neutron star along with a unique identifier and simulation parameters. Keyword and numerical range based search and sorting facilities are provided by proprietary JavaScript code on the website. The data for individual simulations can be downloaded. Metadata is provided in custom ASCII files based on the NRAR format. Simulation data is available as custom HDF5 format files stored in a Zenodo instance hosted by Caltech library. Example scripts to read these files are provided via GitHub [24].

Computational relativity (CoRe). The CoRe catalog [13, 25] of waveforms consists of 367 binary neutron star merger simulations. The catalog is organized as a set of individual simulations in a 12-dimensional parameter space, including initial parameters of binary neutron stars and remnant black hole or neutron star along with a unique identifier and simulation parameters. Keyword based search and sorting facilities are provided by proprietary JavaScript code on the website. The data for individual simulations can be downloaded. Metadata is provided in custom ASCII files defined on the catalog website. Simulation data is available as custom HDF5 format files stored in a GitLab instance hosted at one of the CoRe collaborators' institution.

2.2. Generic repositories

Recognition of data as valid research products and the need to provide ways to share data and track academic credit for data products have lead to the development of data sharing solutions on both the institutional level and spanning institutions. Data retention policies adopted by funding agencies [26] have furthered this development. In this section, one international, one institutional, and one federated (national) platform is introduced, respectively.

Zenodo. Zenodo [2] is a general purpose open source [27] research publishing infrastructure and repository developed under the European OpenAIRE program and operated by CERN. It allows researchers to upload, and share all forms of research outputs such as data sets, research software, reports, and any other research related digital artifacts. Each data set is owned by a single user and fine grained access control is not provided. Upon publishing, a digital object identifier (DOI) is minted and assigned to the scholarly record. Keyword based search functionality is provided by Zenodo and individual submissions or individual files in submissions can be downloaded.

Illinois Data Bank (IDB). The IDB [15] is a proprietary institutional data repository which provides access to Illinois research data. IDB allows individual researchers to upload, and share all forms of research outputs such as data sets, research software, reports, and any other research related digital artifacts but does not allow to restrict access to a subset of users. Upon publishing, a DOI is minted and assigned to the scholarly record. Keyword based search functionality is provided by IDB and individual submissions or individual files in submissions can be downloaded. Uploads are limited to researchers at the University of Illinois, while downloads are available to all researchers.

Federated Research Data Repository (FRDR). FRDR [28] is a proprietary platform for Canadian researchers to deposit and share digital research data and to facilitate discovery. Being a federated design FRDR supports fine grained access control to data sets. Upon publishing, a DOI is minted and assigned to the scholarly record. FRDR provides keyword based search functionality. Uploads are limited to Canadian researchers, while downloads are available to all researchers.

2.3. DataVault

By combining advantages from domain-specific and generic data platforms, we design, develop and deploy a domain-specific data repository for sharing and archiving NR simulation data, featuring collaboration, open data and open science and meanwhile promoting FAIR [29] (findability, accessibility, interoperability, and reuse) data principles. The following section discusses how features of DataVault ensure it provides each of the desired features mentioned in table 1.

3. DataVault description

DataVault is built by and initially for the Einstein Toolkit community. Its design is based on the community's needs as shown by its key features in table 1. This section gives a high-level overview of DataVault's structure and functionalities, as well as how the functionalities are applied to different use-case scenarios.

3.1. Architecture and workflow

DataVault is implemented as a web-based application connecting to a storage and search engine. Its user interface provides easy management and discovery of data sets. This section describes architecture and design features in detail.

Data access, processing and storage are among the most critical factors when developing a research data repository [30]. When users upload data sets, DataVault processes them through multiple pipelines, which include metadata extraction, and collection assignment. Structure and workflow of the DataVault is shown in the figure 1.

To advance open science and ensure wider distribution, DataVault is developed based on the open-source data analytics platform *Girder* [31]. Girder includes basic functionalities, such as data set upload and download, collection creation, user group assignment and registration control. Girder can be divided into two components: the core and plugins. The core component of Girder implements the fundamental framework for both the user interface front-end and server back-end. It constructs the critical API endpoints to let additional plugins provide features and acquire information, via event triggers such as 'upload' and 'new user registration'. All extended functionality is implemented as Girder plugins. In general, a plugin is composed of front-end and back-end parts. The front-end is implemented using JavaScript and serves as an interface between the user and the back-end. The back-end is implemented using Python, it handles requests sent by the front-end and makes API calls to retrieve the information from the core component and process them.

Girder is chosen because it has a complete set of the functionalities required to effectively build the data repository with desired features. Girder is designed with security and extensibility in mind via the separation into core and plugin components. Therefore, research groups using DataVault can implement new features as additional plugins to Girder. Furthermore, Girder provides detailed documentation and has an active user community for discussion and support, and is actively developed and maintained.

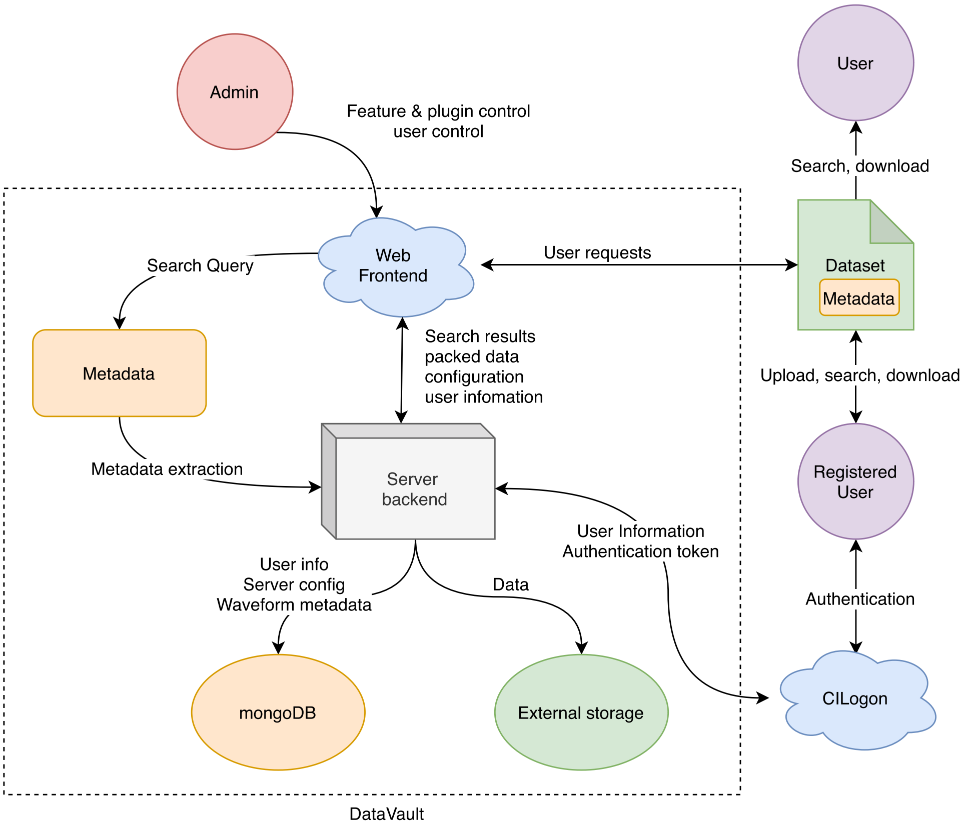


Figure 1. DataVault structure and workflow. DataVault components are enclosed within the black box. All interactions are indicated by arrows. Users are authenticated using CILogon, and only then can they upload data sets from DataVault. When a user uploads the waveform, the metadata is extracted on the server side and stored in MongoDB. All data and metadata is stored in external storage to preserve the data in case the Docker image needs to be rebuild. Users can send search queries either using the web user interface or a command line interface. The server parses the search query, retrieves and returns the requested information to user.

DataVault is implemented as a set of Girder plugins. These plugins include metadata extraction, advanced metadata search, and CILogon as an extension to the existing OAuth 2 login plugin.

Metadata extraction. Metadata describes simulation data sets. The metadata fields in the table 2 are critical to waveform data sets. They specify physical initial conditions for the simulation, such as masses, initial separation and initial orbital velocity which are key parameters of interest to waveform modellers and numerical relativists. Although there is no standard file format accepted by all the NR community yet, the LIGO collaboration defined a file format as part of the NRI infrastructure [19]. DataVault's built-in metadata extractor support this NRI format and provides search functionality based on it. Details of this data format, including the explanations of metadata attributes and rationale for establishing this data format are discussed in [19].

These metadata attributes define the simulation, as they are the physical initial conditions for the simulation. For Einstein Toolkit, users need to write a parameter file to set up the simulation

Table 2. NRI [19] format metadata fields understood by DataVault. Spin 1, spin 2, LNhat, nhat are 3D vector quantities and have a separate metadata field for each x, y, z component. More details on these parameters can be found in [19] section 2.3.

Attribute name	Physical parameters	Type	Range
Mass 1 (M_1)	Mass of more massive object	Float	$[0, \infty)$
Mass 2 (M_1)	Mass of less massive object	Float	$[0, \infty)$
eta (η)	The symmetric mass ratio	Float	(0, 1]
Spin 1 x, y, z ($\chi_{1,(x,y,z)}$)	Dimensionless spin vector of object 1 in NR frame	Float	
Spin 2 x, y, z ($\chi_{2,(x,y,z)}$)	Dimensionless spin vector of object 2 in NR frame	Float	
LNhat x, y, z ($\hat{L}_{n,(x,y,z)}$)	Newtonian orbital angular momentum unit vector	Float	
nhat x, y, z ($\hat{n}_{(x,y,z)}$)	The orbital separation unit vector	Float	$[-1, 1]$
Omega (MΩ)	Dimensionless orbital frequency	Float	$(0, \infty)$
Eccentricity (e)	Estimated eccentricity	Float	[0, 1]
mean_anomaly	Estimated mean anomaly	Float	-1 for N/A, [0, 1]

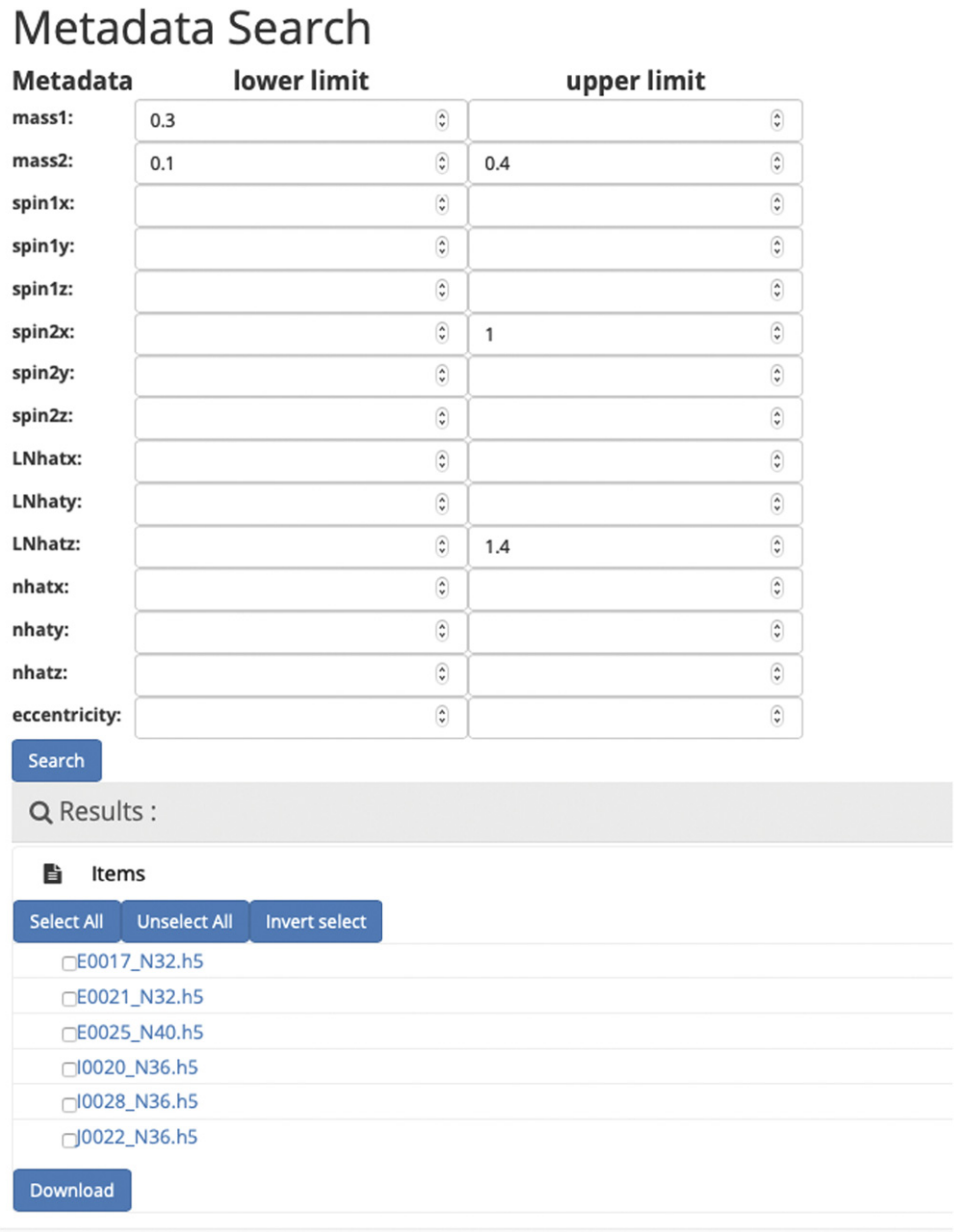
with evolution methods, diagnostics, and initial data. The metadata in table 2 are the parameters for the simulation.

The set of metadata also contains a user chosen identifier for the waveform. DataVault provides extensive support for metadata presentation and extraction. When a user uploads waveforms, DataVault automatically extracts metadata from the uploaded files and verifies the format of the metadata to ensure it adheres to NRI format [19] specifications. As a domain-specific data repository with known metadata, DataVault offers advanced semantic search functionality, which is introduced in the next paragraph.

Search plugin. To help users find waveforms more efficiently, DataVault provides an advanced search plugin. Users search for waveforms using the metadata fields shown in table 2. When searching, users specify a numerical range for the metadata attributes they are interested in. If a lower limit or upper limit not given, then the search assumes it to be unrestricted. Users can immediately see search results and download either all or a subset of the waveforms from within the result display. Figure 2 shows the search user interface and results display.

CILogon based authentication. To ensure only authorized users can upload data and access private data, authentication plugins require community users to log. DataVault primarily relies on CILogon for institutional logins. CILogon is developed for academic users, it allows users to use their institutional credentials to log in without needing to create a separate DataVault account. Thus DataVault benefits from trust in the identities reported by CILogon. As an example this allows a research group to easily grant access to new members without having to perform their own identity verification. Generic Oauth2 login, such as GitHub and BitBucket, is also supported for external collaborators whose home institutions are not participating in CILogon. An additional layer of access control enables that administrators approve access of registered users before new users can upload data.

Data set collections. DataVault is a platform for sharing data, including published data and private data for ongoing research. To facilitate these goals, DataVault supports creating data collections consisting of multiple data sets. Access to all data sets in a collection is controlled at the collection level which provides a convenient way to organize related data sets. For example research groups that share data among members, can create data collections and grant access to their group members only but none other. In this way, data stored online remains private to the research group. Collections also organize data sets into categories to simplify searching for and downloading of data sets matching common criteria.



Metadata Search

Metadata	lower limit	upper limit
mass1:	0.3	
mass2:	0.1	0.4
spin1x:		
spin1y:		
spin1z:		
spin2x:		1
spin2y:		
spin2z:		
LNhatx:		
LNhaty:		
LNhatz:		1.4
nhatx:		
nhaty:		
nhatz:		
eccentricity:		

□E0017_N32.h5

□E0021_N32.h5

□E0025_N40.h5

□I0020_N36.h5

□I0028_N36.h5

□J0022_N36.h5

Figure 2. Search plugin user interface. Users input lower and upper limit in the search box. The results section shows all waveforms with metadata values within the specified numerical range. Users then select individual ones or all waveform files for download.

3.2. Deployment

DataVault is containerized to achieve portability and speed up deployment. Containerization is achieved using Docker [32], which is open-source, lightweight and portable. Both the Dockerfile used to build the DataVault image and the docker-compose file to build the full server infras-

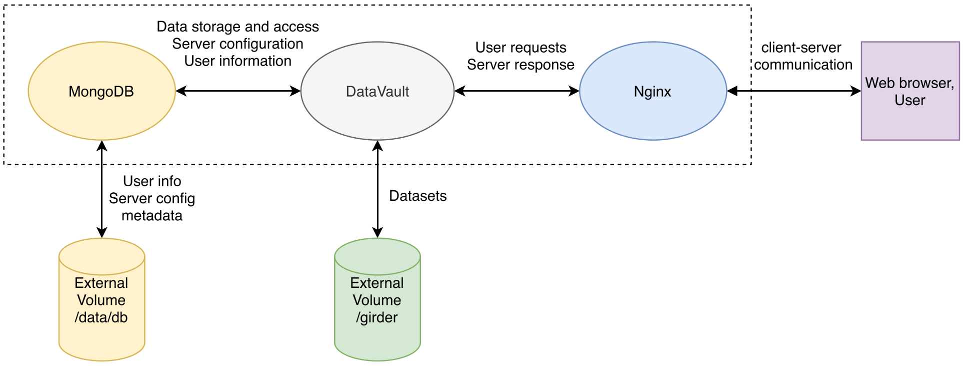


Figure 3. DataVault container setup. Each ellipse represents a container. Users communicate with the Nginx container which forwards requests to the DataVault container. MongoDB also resides in a separate container. All data and configuration files are stored outside of the containers.

tructure consisting of DataVault, MongoDB [33] and Nginx [34] are available for download [4]. Figure 3 shows the interaction between the components.

The MongoDB volume is mounted externally for data persistence since data stored in the container is destroyed when the container stops running. Thus, in case the server operation is interrupted and the running docker container is shut down, the external mounting volume can preserve the server configurations, users information and the data set stored in the DataVault.

3.3. DataVault use-cases and application

DataVault's features described above target multiple scenarios, and three hypothetical examples are provided in this section to illustrate some use-cases for the application of DataVault into different research tasks.

For NR and waveform modeling communities. DataVault directly benefits groups using the Einstein Toolkit, both as producers of waveform data sets and consumers of these data sets. Einstein Toolkit users can store the data using the DataVault instance hosted at NCSA. These users store waveforms generated for published papers, as using the unique PIDs generated for data set provenance and citation. A sample set of 89 waveforms generated by the NCSA gravity group serves as a demonstration for how data sets can be arranged in collections. Ownership of the data sets is shared among all NCSA gravity group members with access controlled by DataVault. Non-NCSA groups interested in this data sets access it using read-only permission. DataVault's advanced search functionality immediately provides a convenient means for groups modeling gravitational waves using semi-analytical methods to select and download numerical waveform data sets for calibration and testing of their models.

For numerical astrophysics community. A DataVault instance is hosted at NCSA for public use and other research groups can choose to self-host a DataVault instance to store data locally. They use the collections to group data sets of interest and share access to the collections among group members. On the other hand, numerical groups whose data sets are not supported by public DataVault instances, or who desire a 'branded' instance of DataVault, make use of the open-source nature of DataVault to access the source code and modify it to accommodate their needs. The metadata of waveforms in DataVault currently are the NRI format [19]. Research groups can adapt metadata extraction and advanced search functionality to their needs. DataVault's modular design make it easy to modify the metadata extraction and the search code according to the structure and format of the data sets.

For public and education use. Data stored in NCSA's DataVault instance is open for public us. For students and instructors at institutions without a numerical astrophysics research program, or even for high-school educators, DataVault provides a way to access research data produced by supercomputing simulation. An instructor uses DataVault to select data for their students to work, restricting access to the collection to their respective class. Student upload simulation results and share them among themselves.

4. Sustainability

DataVault is maintained by the Einstein Toolkit team at NCSA and there is a path for the platform to be supported by the Einstein Toolkit community as DataVault gains users. This section discusses the future plan for DataVault and how it will be supported in different phases of the operation as part of the Einstein Toolkit.

DataVault's future development is an iterative process consisting of two alternating phases: development phases and maintenance phases. Each of these phases defines a set of objectives for DataVault. Although there is no clear boundary between each phase, goals and objectives for each phase are individually specified below.

Development phase. In this phase, we focus on developing new functionality and features for DataVault. This includes developing new plugins, A/B tests and gathering user feedback for further improvement and optimization.

Maintaining phase. The main objective of this phase is to keep the production DataVault in normal operation, and provide users with access to data. The team will not be developing some new features during this phase, and instead gather feedback from users and discuss for further possibilities.

4.1. Extensibility

DataVault builds on Girder, meaning that additional features can be easily implemented by modifying the plugins, as discussed in section 3. DataVault's source code repository [4] contains full developer's documentation of the existing plugins, considerably simplifying the task of adding new Girder plugins. DataVault being licensed under an open source license, the existing plugins serve as a starting point.

4.2. Future work

In the future we plan to add new features and optimization of current features based on community feedback. We plan to add more detailed online visualization, such as waveform plots and metadata visualization. DataVault's search functionality is key to its use and we will extend it to allow for user defined queries and more complex combinations of search terms. This will be an extension to the current advanced search functionality.

5. Conclusion

In this work, we presented a domain-specific data repository, DataVault, to facilitate collaborations by sharing data among relativity research groups and a wider non-scientists audience. To inform the fundamental framework design and collect necessary features for a potential data repository in NR community, a comparative review of 8 existing data repositories was conducted. 5 of the repositories are domain-specific and the other 3 are generic. We summarized their capabilities and compared them using a set of criteria that are necessary for research work in the numerical astrophysics community.

In the comparative study we found that there was currently no single repository with all the features useful to the numerical astrophysics community. Using the information collected in the study, we designed and developed a data repository, DataVault, that provides the identified features. An overview of DataVault's architecture, deployment and extensibility was provided. To illustrate the usefulness of DataVault, we investigated three use cases and discussed how DataVault can be applied in each scenario. We conclude that DataVault enables an efficient, multi-purpose data sharing process for data intensive projects.

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Data availability statement

The data that support the findings of this study are openly available at the following https://datavault.dev.ncsa.illinois.edu/.

Appendix A. Waveform catalog

To illustrate use of DataVault and speed up its adoption by the Einstein Toolkit community we added the catalog of 89 eccentric NR simulations reported in [36] supplemented by an eccentricity measurement using the method presented in [37]. Waveforms were postprocessed using `SimulationTools` [35], and converted to NRI file format [19].

This waveform catalog consists of non-spinning binary black hole merger waveforms with mass ratio $1 \leqslant q \leqslant 10$ and eccentricities $0 \leqslant e_0 \leqslant 0.18$ at fifteen waveform cycles before merger and contains multipolar modes up to $\ell = 4$. All simulations used the Einstein Toolkit [5] using parameter files based on [38].

DataVault makes all metadata stored in the HDF5 files accessible and searchable through its user interface and allows subsets of the catalog to be downloaded.

The catalog data set serves as a real world test case for DataVault's usability as a waveform repository for the numerical astrophysics community.

- Waveforms were produced by multiple members of the NCSA gravity group, making use DataVault user and group management functionality when controlling access to the data set while it was being prepared.
- The large number of files require automatic extraction of metadata, describing the numerical simulations.

- The multi-dimensional parameter space spanned by mass ratio and eccentricity makes it possible to define non-trivial subsets for example by selecting all circular waveforms or a sequence of increasingly eccentric waveforms for a fixed mass ratio.
- These waveforms are of interest to the larger GW modelling community, with potential users outside of the research group at NCSA, thus demonstrating the usefulness of community repository.

Appendix B. Eccentricity estimation and extraction

The eccentricity of the NR simulations waveforms were extracted using the algorithm specified in [37]. The algorithm found the eccentricity by passing the initial guess of the eccentricity through a coarse search and then followed by a fine search. We modified the code by adding a Newtonian initial guess for the eccentricity, based on the initial parameters from the metadata file created in each simulation. These parameters include the initial positions ($\vec{r}_1, \vec{r}_2$), initial linear momentum ($\vec{p}_1, \vec{p}_2$), and initial ADM mass (m_1, m_2). By using classical orbital mechanics, the Newtonian initial guess for eccentricity is:

$$e_0 = \sqrt{1 + \frac{2E_{\text{sp}}h_{\text{sp}}^2}{GM}} \tag{B.1}$$

where E_{sp} and h_{sp} are the specific energy and specific angular momentum respectively, defined as

$$E_{\text{sp}} = \frac{1}{\mu}\left(\frac{\|\vec{p}_1\|^2}{2m_1} + \frac{\|\vec{p}_2\|^2}{2m_2} - \frac{Gm_1m_2}{\|\vec{r}_1 - \vec{r}_2\|}\right) \tag{B.2}$$

$$h_{\text{sp}} = \frac{\|\vec{h}_1 + \vec{h}_2\|}{\mu} \tag{B.3}$$

$\vec{h}_1$ and $\vec{h}_2$ are the angular momentum of the two objects. These eccentricities were added to the metadata of the waveforms and presented online on the DataVault.

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