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The GHGA Archive: Selected Updates

Conceptualisation, Implementation, and Discussion

Jens Krüger*, Jordy Didier Orellana Figueroa,
Zehra Hazal Sezer, Thomas Jakob Zając
High Performance and Cloud Computing Group
Eberhard Karls Universität Tübingen
Tübingen, Germany
*jens.krueger@uni-tuebingen.de

Kersten Breuer, Luiz Manoel Rocha Gadelha Junior,
Christoph Zwerschke
GHGA Office
German Cancer Research Centre (DKFZ)
Heidelberg, Germany

Bilge Sürün
Applied Bioinformatics
Institute for Bioinformatics and Medical Informatics
Eberhard Karls Universität Tübingen
Tübingen, Germany

Sven Nahnsen
Quantitative Biology Center
Eberhard Karls Universität Tübingen
Tübingen, Germany

***Abstract*—The German Human Genome-Phenome Archive (GHGA) is a cross-institutional project and German National Research Data Infrastructure (NFDI) consortium for the development of a scientific gateway for secure omics data sharing based on FAIR principles to act as the German node of the federated European Genome Archive (fEGA), participating also in the European Genomics Data Infrastructure (GDI) project. Started in 2020, the GHGA is reaching its first major release milestone: having released an online science gateway for metadata browsing termed the Metadata Catalog, the next step involves the development of a portal that extends the functionality already available to also include authentication, data download (via an external tool), and data access request management: the GHGA Archive. We present here a brief overview of the new technologies and functionalities that will be available for the Archive version of the GHGA science gateway.**

Keywords—human genome data, omics, science gateway, FAIR, sensitive data, NFDI, FEGA

I. INTRODUCTION

The German Human Genome-Phenome Archive (GHGA) is a multi-institution project that seeks to develop a scalable and secure omics data sharing gateway for Germany, as well as an ethical and legal framework to handle omics data in a data-protection-compliant but also open and FAIR manner [1], a harmonised metadata schema, and standardised workflows to process all incoming omics data. GHGA is part of the German National Research Data Infrastructure (NFDI) [2, 3], and has 21 partner institutions in genomic medicine and bioinformatics. The GHGA infrastructure is organised in seven distributed data hubs (in Heidelberg, Tübingen, Munich, Dresden, Cologne, Berlin, and Kiel), all centrally coordinated at the German Cancer Research Centre (DKFZ) in Heidelberg (GHGA Central). GHGA acts as the German node for Europe-wide initiatives such as the federated European Genome-Phenome Archive (fEGA) and the European Genomics Data Infrastructure (GDI). GHGA seeks to shape future international data-sharing standards and contribute to a sustainable data infrastructure worldwide.

There are several phases planned as milestones during the development of the GHGA platform. The phase currently in development is the GHGA Archive, with the next being the Atlas and Cloud phases. Amongst their many features, Archive will act as the fully functional national EGA node for Germany, while Atlas will provide researchers the possibility of executing standardised omics analysis pipelines through a singular GHGA gateway, and Cloud will allow for large-scale cloud-based data analysis in the modality of a Platform as a Service (PaaS).

However, in addition to the future milestones described above, a preliminary metadata browsing platform has already been released as the GHGA Metadata Catalog, the first version of the GHGA science gateway [4].

A. The GHGA Metada Catalog

The GHGA Metadata Catalog [5] was released in 2023 and serves as a discovery platform for human omics data that is available for research purposes. The platform allows users to browse, search, and filter metadata submitted to GHGA. Currently, the metadata for 82 datasets from eight studies are available for browsing (from a total of 62 at release). Five of the studies are available in the EGA catalogue, with the remaining three shared by our partners with GHGA.

The GHGA Archive phase provides additional features on top of those currently available in the Metadata Catalog. We discuss in the next sections some of the many features and technologies that will be available for the release of the GHGA Archive, highlighting especially those additions to the Metadata Catalog.

II. COMMUNITIES AND STANDARDS

A. EGA and GDI Integration and Workflows

GHGA is the German node in both the Federated EGA [6] and the European Genomic Data Infrastructure (GDI). Therefore, our roadmap includes integrating GHGA's microservices with FEGA and GDI. In particular, GDI makes available the Starter Kit [7], a collection of software components that can be used for deploying a node in the infrastructure. These components include, for instance, the Beacon v2 service [8] for data discovery, the Life Science Authentication and Authorization Infrastructure (LS AAI) [9], the Resource Entitlement Management System (REMS) [10] for managing data access requests, and the Sensitive Data Archive [11].

GHGA independently implemented equivalent functionality in its microservices, but both follow standards from the Global Alliance for Genomics & Health (GA4GH), such as Crypt4GH [12] and Data Repository Service (DRS) [13] which should facilitate their integration. As a first step toward integration, an instance of the Beacon v2 service was deployed in GHGA and standardised workflows for ingesting data into the service are being discussed, which include processing data for calling variants and mapping data and metadata to the Beacon data model. The instance of Beacon at GHGA will be visible in the centralised GDI Beacon Network user interface, in which users will be able to perform federated queries across the existing Beacon v2 instances in different GDI nodes across Europe following data privacy and access control constraints.

GHGA is building upon the nf-core and nextflow community [14] to build, maintain, and analyse NGS analysis workflows for all incoming data modalities such as nf-core/SAREK [15], as well as creating runtime configurations for each data modality with stable identifies, and continuously evaluating their performance. In collaboration with the nf-core community and beyond, GHGA is maintaining and co-developing six workflows. To evaluate the performance of the workflows GHGA together with the German NGS Competence-Network developed a continuous benchmarking framework: NCBench [16]. GHGA is also creating a runtime configuration to uniformly process NGS data while guaranteeing the highest standards and quality of the workflows.

By maintaining scalable, reproducible, and continuously benchmarked workflows, GHGA will create a harmonised and standardised NGS data resource ready to be used by the German research community. Such a harmonised resource will enable cross-analysis of projects and population-scale studies, promote new collaborations, and research projects, and establish the foundation for developing a German-based variant frequency database.

B. Ethical, Legal, and Social Implications (ELSI)

Due to the highly sensitive nature of the data involved (individuals' omics data), strong data protection measures have been developed for the GHGA. Informed consent from the individual is always required for their data to be used for research purpose. For this purpose, the Ethical, Legal, and Social Implications (ELSI) team of GHGA has developed *consent modules*: standardised text fragments for researchers to adopt in their patient or participant consent forms [17]. These consent modules provide researchers a set of templates that provide individuals with clear and unambiguous information on what will happen to their data if they consent to their sharing. These measures are only but a small part of the many ways [18] GHGA complies (as a data processor) with the General Data Protection Regulation (GDPR) regulations [19], along with measures such as the pseudonimysation of the data shared, and compliance with the 'right to erasure' (Art. 17).

Moreover, the legal relationships between the various entities that operate GHGA (e.g. between GHGA Central at the DKFZ in Heidelberg and the GHGA data hubs in other institutions [20]), as well as those entities that submit data and metadata (i.e. to the Metadata Catalog) to GHGA are defined by a series of legal documents available online [18].

C. The GHGA Metadata Schema v. 1.x

The GHGA Metadata Catalog implemented an earlier version of the GHGA Metadata Schema (v. 0.8) defined in LinkML. Since then, a new major release has been made public [21]. This new schema (version 1.0 and above) has a "Submission" entity as the root class of the model that references all other model entities (e.g. *Dataset, File, Sample*). This new design embodies a connected graph structure, facilitating seamless navigation between various classes. This strategic approach enables backend microservices to efficiently interact with the data by leveraging these interconnected relationships.

GHGA Metadata Schema v1.x has considerable differences from the EGA metadata schema. However, the conversion between both models nevertheless remains possible, as the backend microservices that process the metadata for the GHGA Archive perform (meta-)data *transformations* that could convert to and from the EGA schema. EGA to GHGA metadata transformation is currently not yet implemented, but there already exists a conversion strategy developed for this purpose, and compatibility should not be an issue.

This new major version of the Metadata Schema is currently in use for the Archive.

III. TECHNOLOGY

A. Schemapack and Datapack

To describe and validate structural requirements with respect to metadata, we needed a rich schema language. JSON Schema is an industry-standard commonly used for such purposes. However, to reduce redundancy and ensure consistency, the naturally complex relations in scientific and medical metadata are best modelled in a normalised fashion which is not supported by JSON Schema on its own. To this end, we devised a specification and associated tooling called schemapack that allows the creation of normalised relational data models on top of JSON Schema. Thinking of linked data in terms of entity-relationship models, a clear separation of concern is applied: JSON Schema is used to describe the (content of) individual entities while schemapack focuses solely on modelling relations between entities. Much like relational database management systems, data normalisation is achieved by establishing relations between entities using foreign key-based references. Schemapack supports modelling all common cardinalities (one-to-one, one-to-many, and many-to-many) as well as the modality of the relations at both ends.

To standardise and simplify the navigation of the relationship graph, we furthermore proposed an additional specification called datapack that imposes a structure for depositing relational data. Applying the same separation between entity content and entity relations, datapack goes hand in hand with the schemapack specification. Thereby, the datapack specification facilitates the interpretation of data with respect to a schemapack model.

The schemapack and datapack specification as well as associated tooling is all publicly available under the Apache 2.0 license [22].

B. *Authentication and Authorisation*

For an archive of human omics data, authentication and authorisation of users who want to access datasets are crucial features of the system. For authentication, the GHGA Archive uses the Life Science Login (LS Login) [23] authentication service from EOSC-Life [24]. This allows researchers to login to the GHGA data portal in the web browser using their institutional user accounts. For authorisation, the GHGA Archive makes use of the GA4GH Claims [25] technical standard to define access permissions and assertions about researchers. This allows passing authorisation information in and out of the system via the GA4GH Passport [26] standard, though currently the GHGA Archive only creates and accepts its own GA4GH Claims.

To decouple the system from the OpenID Connect [27] authentication mechanism used by LS Login and from LS Login itself as OpenID provider, a translation layer between the external and internal authentication has been implemented in form of an Auth Adapter service. This service is used by the API gateway to authorise access and translate external access tokens to internal access tokens which can be validated by the internal services independently of the externally used authentication provider. The communication between the API gateway and the Auth Adapter happens via the ExtAuth protocol [28].

The Auth Adapter provides information about which user made a request, and which internal role the user has, via an internal access token. The information by this token can be used by the internal services directly, but the token can also be used to request more detailed access information for a user from the Claims Repository service, which holds the mentioned GA4GH claims about users of the system, particularly data access grants for individual datasets.

Since the actual identification and authentication of users via LS Login happens using the infrastructure of their home organisations, the strength of both identification and authentication can vary depending on how these are implemented there. Particularly, LS Login currently cannot verify or require whether the authentication uses a second factor. Therefore, the GHGA data portal provides its own two-factor authentication on top of LS Login and combines this with a verification of the user via an *independent verification address* (IVA) shared by the external institution. The data access grants are always bound to these IVAs. Users who are logged with a second factor can request verification of an IVA from GHGA. After entering a verification code sent by GHGA via the specified address, the IVA is considered verified so long as the same second factor is used for authentication. Currently, the GHGA portal uses standard TOTP tokens [29] as the second factor. Creation and verification of these tokens also happen inside the Auth Adapter service.

This authentication process allows to securely and reliably authenticate researchers who log in to the GHGA data portal using a web browser. However, since the research data that is accessible in the GHGA Archive is typically too large to be downloaded directly via the web browser, a command line tool called GHGA Connector has been provided to download (and later also to upload) data to the GHGA Archive (see below). In the GHGA data portal, researchers can define which datasets they want to download (either completely or partially), after the necessary data access grants have been given and the associated IVAs have been verified. The GHGA data portal then provides a corresponding download token that allows downloading exactly these files using the GHGA Connector. The download token is also encrypted using the Crypt4GH [12] key of the user. After entering this download token in the GHGA Connector, a download of the Crypt4GH encrypted files can be started.

C. *Infrastructure*

All GHGA microservices provide Docker [30] images for easy deployment. The resulting containers are deployed in a Kubernetes Cluster [31] using computing resources in the de.NBI cloud [32]. GHGA uses separate staging and production environments to verify inter-service interactions before moving new releases to production.

Data is stored in an encrypted state in S3-compatible object storage. Different buckets are used for temporary data during ingress and egress and permanent storage buckets are shielded from outside access.

Choosing S3 as storage solution facilitates federation between GHGA's various nodes, as different compatible implementations exist at the participating facilities, e.g. Ceph or IBM COS.

D. *Front-End*

The Archive broadly shares the same technology stack with the Metadata Catalog [4], both consisting of a TypeScript-based

React front-end and NodeJS server containerised in a Docker image and deployed on a Kubernetes cluster (see above).

Moving forward, however, we plan a complete refactoring of the front-end based on a different tech stack. This is due to the current tool used for our React front-end (*create-react-app*) has become stale and is planned to be completely reworked in the future [33], requiring a complete refactoring in either case. This provided an opportunity to consider alternative frameworks and libraries.

In this reconsideration of technology used, we evaluated several available frameworks, and chose to use Angular [34], another JavaScript Single Page Application (SPA) framework based on TypeScript.

The same functionality will remain available after the migration of the data portal to the new framework; thus, we expect that the information of the next section will not change for the future public versions of the GHGA Archive.

IV. FUNCTIONALITY

In addition to sharing the same technology stack, the Archive currently also inherits the same features as the Metadata Catalog, with important additions.

Users can browse, filter, and search the metadata uploaded to GHGA, as well as request access to the data of a chosen dataset. However, as mentioned above, authentication via LS Login with additional 2FA is now possible and is required to perform many tasks related to data access. Moreover, the online gateway now handles access requests within the site itself, rather than requesting the user to perform the data requests via e-mail. In addition, the GHGA Archive provides users with a token that can be used in an additional GHGA tool to download the data described by the metadata. Uploading is also available for GHGA data stewards through an external tool but will be made available for researchers in the public release.

We describe the details of the new functionality below.

A. Data Access, Download, Upload

The GHGA Metadata Catalog enabled browsing metadata for available datasets but did not yet have the capabilities to interact with the actual omics data. With the GHGA Archive, functionality to request access to and subsequently download datasets has been added (both through the online gateway), and submission of new datasets has been facilitated. To this end a set of microservices and two command line tools have been developed.

To download data from GHGA, access for a selection of files first must be requested through an online form available to logged in users when browsing dataset metadata in the data portal for Archive. If the request is approved by a data steward through the access request management page in the same data portal, a work package containing all necessary information for the download process is created internally in the Work Package service. The data requester gets an encrypted access token with a limited lifetime that is used with the GHGA Connector command line tool.

The token is decrypted by the Connector download command, exchanged for the necessary work package information, and used to retrieve work order tokens that are used to authorise the actual file downloads and have a very brief lifetime. In the next step, each file is requested from the Download Controller Service which initiates staging of the requested file to an S3 bucket from which the file is then downloaded. This is done to shield the permanent storage location from direct access. Successfully downloaded files are encrypted and need to be decrypted by using a separate decrypt command that is also provided by the Connector [Figure 1].

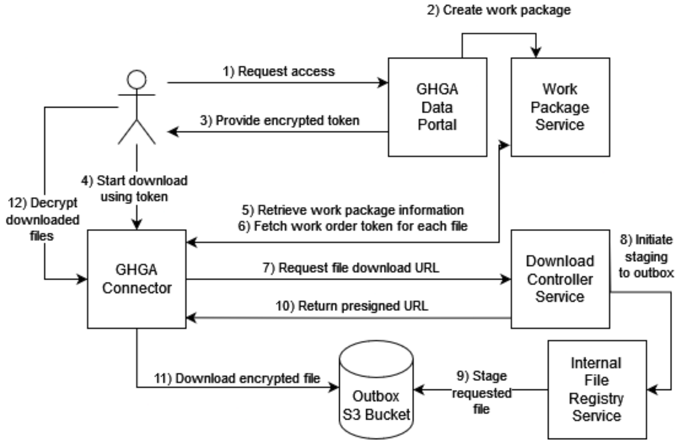

Figure 1. Diagram of the download process. Steps 6–11 are repeated for each file.

The upload of datasets contained in a submission is restricted to data stewards in the first release of GHGA Archive, but later releases will allow a broader audience to use the same Connector CLI tool that is being used for download. In the meantime, upload is currently implemented as a two-step process in a separate CLI tool called the Data Steward Kit. First, files are encrypted using Crypt4GH [12] and uploaded to an intermediate S3 bucket. After successfully uploading the encrypted file, the encryption secret is transferred to a HashiCorp Vault [35] via the File Ingest Service and the corresponding secret ID is returned. A JSON file containing all relevant information is produced for each uploaded file locally. After all uploads have finished, a separate command of the Data Steward Kit is used to ingest the information from the JSON files into the Internal File Registry Service via the File Ingest Service. This also triggers the files to be moved to permanent storage [Figure 2].

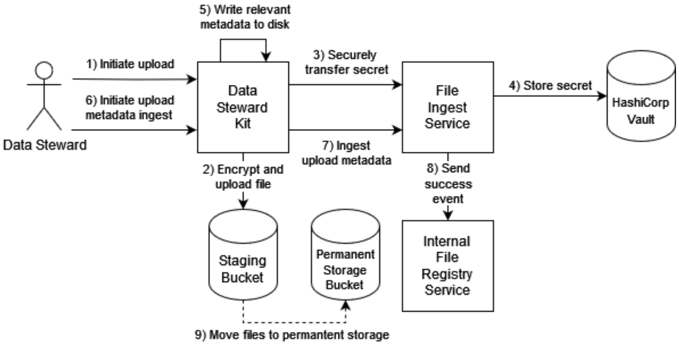

Figure 2. Diagram of the upload process. Steps 1–5 and 8-9 are repeated for each file.

B. Login, Profile, and 2FA Management

To be able to request or download data, users must first have logged in via LS Login in the online gateway, and – if registering for the first time – register to the GHGA data portal and set up two-factor authentication via an authenticator app. In addition, an independent verification address (IVA) must be made before any data can be requested or downloaded. These are created via the user profile page. The verification process is initiated by the user, who waits for the data steward to send a verification code in one of the four options chosen by the user for verifying their identity (SMS, fax, a postal letter, or in person).

The user requests access to data on the data portal (see above) and ties this access to a specific IVA. If the user deletes the related IVA, they lose access to the dataset and access must be granted again as a new request.

The data steward has access to additional pages to manage incoming data access requests, as well as managing user IVAs (e.g. processing IVA verification, manually un-verifying IVAs).

If the user loses their 2FA authenticator setup and requests a new one, all existing verification addresses are reverted to the unverified status, and the user loses access to requested datasets until they perform the verification process once again, ensuring data access is only possible after the data steward verifies the user identity.

CONCLUSIONS

Considerable new functionality is being developed for the next phase of the GHGA science gateway: the GHGA Archive. Development has been taking place from the back-end to the front-end, with additions such as online data access management, data download and upload tools, metadata schema overhauls, scientific analysis workflows. We have discussed here some of the major changes that have been implemented for the GHGA Archive, as well as how they relate to the already-released GHGA Metadata Catalog.

The release of the GHGA Archive science gateway is planned for summer 2024 and is planned to fully rely on the GHGA Central node at the DFKZ in Heidelberg for its operation, from data submission to sharing and storage, with a subsequent update allowing federation of operations to the other GHGA Data Hubs, and later also submission of data from third parties.

However, the Archive is only one of the major milestones in the development of the GHGA project. The next phases of development consist of the Atlas and Cloud milestones, which will provide the ability to perform data analysis within the GHGA platform itself, which will migrate to a cloud-based platform as a service solution for the last phase of development.

The GHGA science gateway will continue to mature to fulfil its role not only as a local node for the EGA and GDI, but also as a FAIR, data-protection compliant, secure, accessible, and research-friendly human omics science gateway.

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