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The gCube system: Delivering Virtual Research Environments as-a-Service

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HIGHLIGHTS

- A software system enacting the delivery of Virtual Research Environments as a Service.
- Rich array of data management services.
- Data processing and analytics solutions.

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ABSTRACT

Important changes have characterised research and knowledge production in recent decades. These changes are associated with developments in information technologies and infrastructures. The processes characterising research and knowledge production are changing through the digitalisation of science, the virtualisation of research communities and networks, the offering of underlying systems and services by infrastructures. This paper gives an overview of gCube, a software system promoting elastic and seamless access to research assets (data, services, computing) across the boundaries of institutions, disciplines and providers to favour collaboration-oriented research tasks. gCube's technology is primarily conceived to enable *Hybrid Data Infrastructures* facilitating the dynamic definition and operation of *Virtual Research Environments*. To this end, it offers a comprehensive set of data management commodities on various types of data and a rich array of "mediators" to interface well-established Infrastructures and Information Systems from various domains. Its effectiveness has been proved by operating the D4Science.org infrastructure and serving concrete, multidisciplinary, challenging, and large scale scenarios.

1. Introduction

Research and knowledge production practices have been changed in recent decades [1,2]. These changes are induced by developments in information technologies and infrastructures. The changes are impacting the whole research lifecycle – from data collection and curation to analysis, visualisation and publishing. Science is digital, collaborative and multidisciplinary, research communities are dynamically aggregated, working environments conceived to support research tasks are virtual, heterogeneous and networked across the boundaries of research performing organisations. Scientists are thus asking for integrated environments providing themselves with seamless access to data, software, services and computing resources they need in performing their research activities independently of organisational and technical barriers. In these settings, approaches based on ad-hoc and "from scratch" development of the envisaged supporting environments are neither viable (e.g. high "time to market") nor sustainable (e.g. technological obsolescence risk).

The *as-a-Service* delivery model promoted by the Cloud computing [3,4] is a suitable model for providing scientists with the services, infrastructures and environments they are expecting [5]. This model consists in services (*a*) delivered over the Internet

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0167-739X/

rather than provided locally or on-site and (*b*) managed by professional and dedicated providers rather than the primary consumers. This model makes it possible (*i*) for the service provider, to leverage economies of scale to keep developments and operational costs low; (*ii*) for the service consumer, to acquire the services and the capacity needed in an elastic way. The presence of services delivered with the as-a-Service delivery model is potentially reducing the efforts and costs needed to implement research supporting environments yet it is not nullifying neither the efforts nor the costs. Depending on the typologies of service(s) that are made available by service providers, scientists might be requested to implement and operate on their own what is missing to get the research supporting environment they need. In practice, there might be a functional mismatch between scientists' expectations and service providers' offerings. For instance, in the case of Infrastructure-as-a-Service, scientists (actually, technical staff supporting them) are supported in the creation of virtual machines (compute, storage, networking) yet they have to install and configure on their own the software they need.

The consumption of the available services and their exploitation to realise the scientific workflows should be an easy task that does not require extra skills nor distract effort from the pure scientific investigation (long learning curves, "entry barriers"). Science Gateways (SGs) [6] and Virtual Research Environments (VREs) [7] have been proposed to close the gap between service providers' offerings and scientific communities' expectations. Very often SGs/VREs are ad-hoc portals built to serve the needs of a specific community only. The development of such environments aiming at facilitating scientists tasks is challenging from the system engineering perspective. Several technologies and skills are needed [8,9]. Moreover, (*a*) people having the requested expertise (mainly expertise related with IT) are not always available in the scientific contexts calling for VREs, and (*b*) technology is in continuous evolution thus offering new opportunities for implementing existing facilities in innovative ways or integrating innovative facilities in existing VREs. This should discourage scientific communities from building their own solutions. Rather it should suggest them to outsource the task of developing and operating Virtual Research Environments to providers delivering them with the as-a-Service model.

This paper gives an overview of gCube.[1] gCube is a software system specifically conceived to enable the creation and operation of an innovative typology of e-Infrastructures, i.e. *Hybrid Data Infrastructures*, that by aggregating a wealth of resources from other infrastructures offers cutting-edge *Virtual Research Environments as-a-Service*. gCube complements the offerings of the aggregated infrastructures by implementing a comprehensive set of value-added services supporting the entire data management lifecycle in accordance with collaborative, user friendly, and Open Science compliant practices. gCube supports the D4Science.org infrastructure that hosts hundreds Virtual Research Environments to serve the biological, ecological, environmental, social mining and humanities communities world-wide.[2] Overall, the VREs are connecting more than 6000 scientists spread all over the world.

2. gCube System Overview

In order to offer VREs as-a-Service, the gCube system has been designed according to a number of guiding principles described below.

Component orientation. gCube is primarily organised in a number of physically distributed and networked *services*. These services offer functionality that can be combined together. In addition, it consists of (*a*) auxiliary components (*software libraries*) supporting service development, service-to-service integration, and service capabilities extension, and (*b*) components dedicated to realise user interfaces (*portlets*) facilitating the exploitation of one or more services.

Autonomic behaviour. Some components are dedicated to manage the operation of a gCube-based infrastructure and its constituents, e.g. automatic (un-)deployment, relocation, replication. These components realise a middleware providing the resulting infrastructure with an autonomic behaviour that reduces its deployment and operation costs.

Openness. gCube supplies a set of generic frameworks supporting data collection, storage, linking, transformation, curation, annotation, indexing and discovery, publishing and sharing. These frameworks are oriented to capture the needs of diverse application domains through their rich adaptation and customisation capabilities [10].

System of systems. gCube includes components realising a rich array of mediator services for interfacing with existing "systems" and their enabling technologies including middlewares for distributed computing (e.g. EMI [11]), cloud (e.g. Globus [12], OCCI [13]) and data repositories (e.g. OAI-PMH [14], SDMX [15], OGC WP*.[3]). Via these mediator services, the storage facilities, processing facilities and data resources of external infrastructures are conceptually unified to become gCube resources.

Policy-driven resources sharing. gCube manages a resource space where (*a*) resources include gCube-based services as well as third party ones, software libraries, portlets and data repositories, (*b*) resources exploitation and visibility is controlled by policies realising a number of overlay sets on the same resource space. This approach is key to have a flexible and dynamic mechanism for VRE creation, since VREs are actually realised through dynamic aggregations of resources.

As a service. The gCube offering is exposed according to the "as a Service" delivery model [3]. The advantage is that the actual management is in the hand of expert operators who manage the infrastructure (*i*) by providing reliable services, (*ii*) by leveraging economies of scale, and (*iii*) by using elastic approaches to scale. Via gCube nodes (servers enriched with microservices) the system offers storage and computing capacities as well as management of service instances (dynamic (un)deployment, accounting, monitoring, alerting). Via gCube APIs the system gives a flexible and powerful platform to which developers can outsource data management tasks. Via gCube services the system offers a number of ready to use applications.

These guiding principles allow providing VREs as-a-Service, i.e. authorised users can aggregate – by using a wizard – existing resources (including data) to form innovative working environments and make them available via a plain web browser or even via a thin client. Of course, the set of resources that can be aggregated cannot be considered sufficient for any exploitation scenario. Whenever a gap between gCube capabilities and user expectations emerges it must be filled by activities ranging from the development of service *plug-ins* adding capabilities to existing components (e.g. for accessing specific data, exploiting a specific protocol, making available a specific analytics method) to the development of new

[1] gCube Software System website www.gcube-system.org.

[2] The list of supported VREs is evolving and it is always available at https://services.d4science.org/explore.

[3] Open Geospatial Consortium Standards and Supporting Documents http://www.opengeospatial.org/standards.

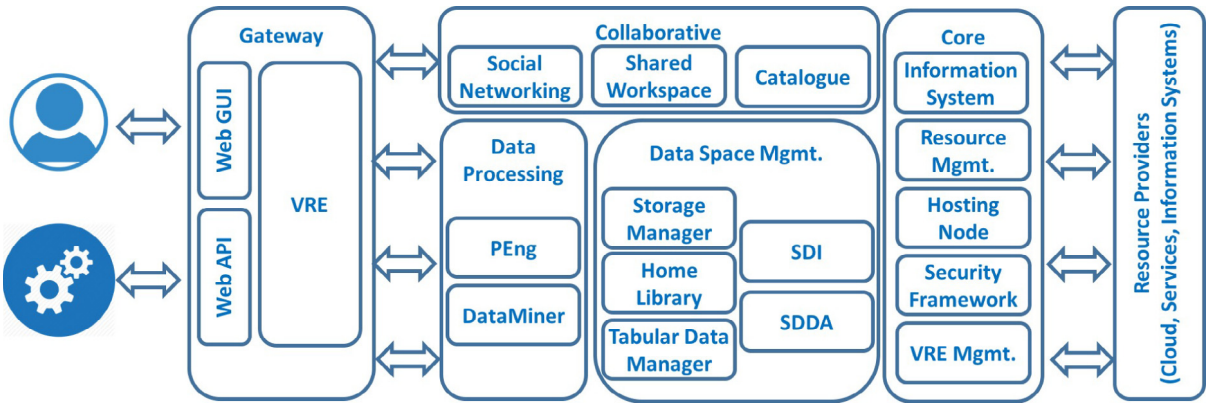

Fig. 1. gCube Functional Areas.

portlets, web apps, or even new services devised to support domain specific workflows.

gCube key components resulting from the above principles are organised according to Fig. 1.

The *gateway* is a portal based on Liferay technology.[4] In the reality the gateway is conceived to be deployed by a number of servers hosting Liferay instances all made available by a proxy guaranteeing high availability and load balancing. The gateway hosts all the portlets implementing GUI components facilitating access to the services. Moreover, for every VRE a proper application context (i.e. a site) is created with the portlet needed by the specific VRE organised according to the specific needs.

The rest of the areas are described in the next sections.

2.1. Core services

gCube core services offer the basic facilities for resources management, security, and VRE management described below.

Resource management. This set of services (Information System, Resource Management Service and Hosting Node) offers facilities for the secure and seamless management (discovery, deployment, monitoring, accounting) of *resources* (proprietary or third party ones) encompassing hosting nodes, services, software and datasets. The *Information System* acts as the registry of the entire infrastructure. It gives global and partial views of the resources and their operational state through query answering or notifications. The *Resource Management Service* is responsible for resource allocation and deployment strategies (e.g. dynamically assigning selected resources to a given context such as a VRE, assigning and activating both gCube software and external software on hosting nodes). The *Hosting Node* is a software component that once installed on a (virtual) machine transforms it into a server managed by the infrastructure and makes it capable to host running instances of services and manage their lifecycle. This type of node can be configured to host a worker service thus making the machine capable to execute computing tasks (cf. Section 2.3).

Security framework. Facilities for authentication and authorisation are supported. They are based on standard protocols and technologies (e.g. SAML 2.0) providing: (*a*) an open and extensible AA architecture; (*b*) interoperability with external infrastructures and domains obtaining Identity Federation (e.g. OpenID). For authorisation, gCube implements a token based authorisation system with an attribute-based access control paradigm. For authentication, users are requested to sign-in with their account (including third-party accounts like Google or LinkedIn). Once logged in, the user is provided with a user token that is transparently used to perform calls on behalf of the user. Whenever a user action implies a call to a service requiring authorisation, the gCube security framework (*a*) automatically collects the credentials to be used by the credential wallet, i.e. a service where the credentials to access each service are stored in encrypted form by using VRE-specific symmetric keys, (*b*) decrypts the user credentials with the specific VRE key, and (*c*) performs the authorised call by passing the credentials and the user token. In this way the connection to the service is established in a secure way while the token is used to verify that the specific user is authorised to call the service.

VRE management. Facilities for the specification (wizard-based) and automatic deployment of complete VREs in terms of the data and services they should offer are supported [16]. These facilities are implemented by dynamically acquiring and aggregating the needed resources, including user interface constituents, from the resource space. This is a very straightforward activity consisting of: (*i*) a *design* phase where authorised users are provided with a wizard-based approach to specify the data and the services characterising the envisaged environment. This is enacted by allowing users to select the items of interest among the available ones; (*ii*) a *deployment* phase where authorised users are provided with a wizard-based approach to approve a VRE specification. Once approved, the deployment starts and the manager is enacted to monitor the automatic deployment of the real components needed to satisfy the specification; and (*iii*) an *operation* phase where authorised users are provided with facilities for managing the user of the VRE and altering the VRE specification if needed. Details on this approach have been presented in previous works [16,17] while a screenshot of the wizard supporting the VRE specification is in Fig. 2.

2.2. Data space management services

Data occupies a key role in science and scientific workflows, thus VREs are called to support their effective management. However, data to be managed are very heterogeneous (formats, typologies, semantics), disaggregated and dispersed in multiple sites (including researchers' drawers), possibly falling under the big data umbrella. In the context of a VRE, it is likely that compound information units are produced by using constituents across the various solutions. To cope with this variety, gCube offers an array of solutions ranging from those aiming at abstracting from the heterogeneity of data (file-oriented and information objects) to those focusing on specific data typologies having different levels of semantic embodiment (tabular, spatial, biodiversity data). Independently of data typologies, all these solutions are characterised by (*a*) support for aggregation of data residing in existing repositories; (*b*) scalability strategies enabling users to dynamically

[4] Liferay website https://www.liferay.com/.

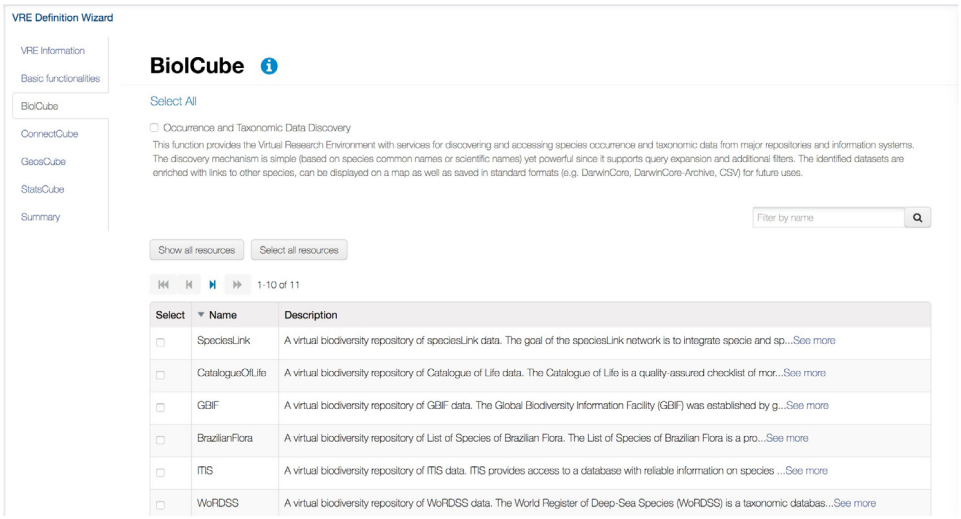

Fig. 2. Virtual Research Environment definition phase: selecting the expected facilities.

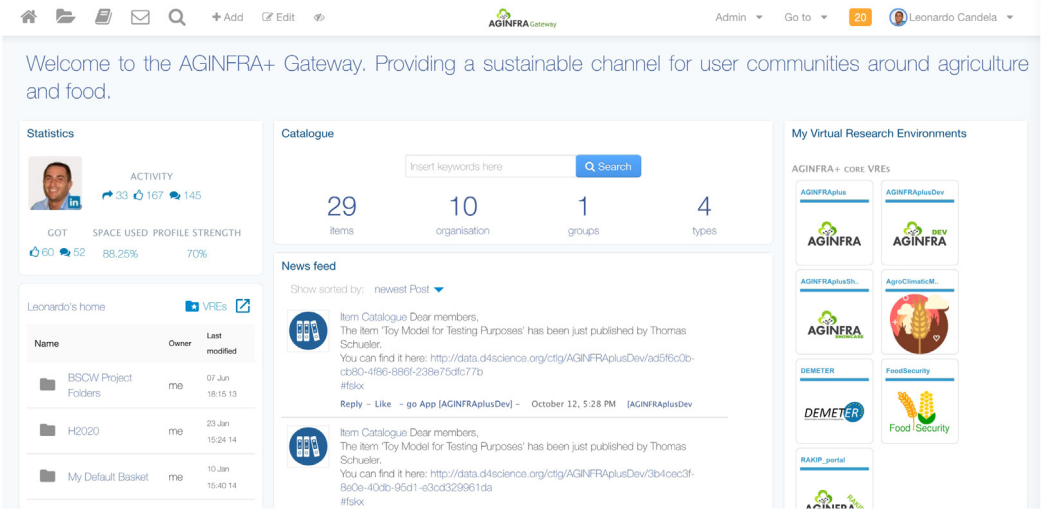

Fig. 3. AGINFRA+ Gateway Home.

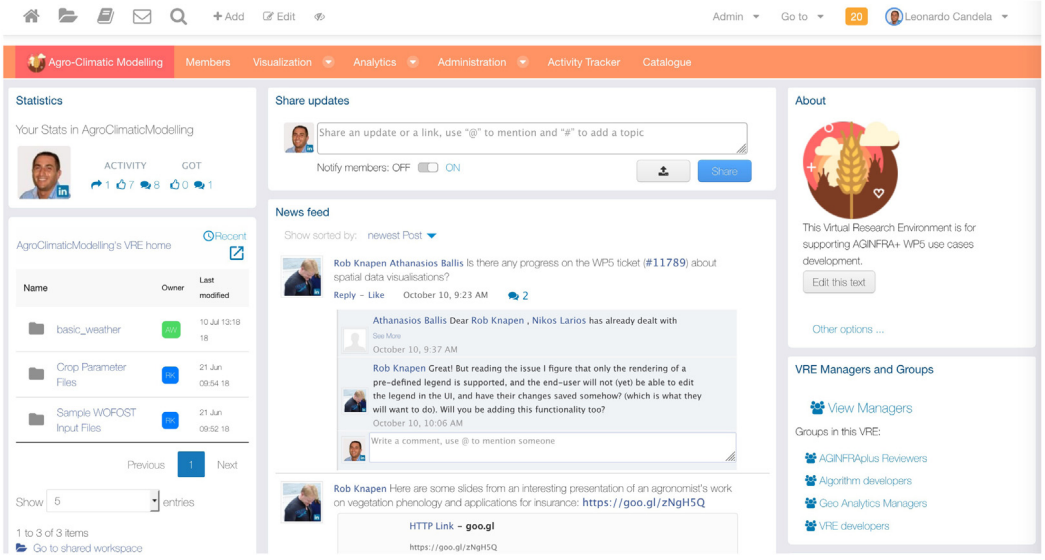

Fig. 4. A typical Virtual Research Environment application.

adding more capacity; (*c*) comprehensive metadata to capture key aspects like context, attribution, usage licences, lineage [18]; and (*d*) policy-driven configurability to adapt the data space to specific needs, e.g. by selecting repositories and datasets. In particular, the following facilities are supported.

File-oriented data. The *Storage Manager* is a Java based software library supporting a unique set of methods for services and applications to manage files efficiently. It relies on a network of distributed storage nodes managed by specialised open-source software for document-oriented databases. In its current implementation, three possible document store systems [19] can be seamlessly used, namely MongoDB, Terrastore and U.STORE [20], while new ones can be added by implementing a specific mediator.

Information objects. The *Home Library* is a Java based software library enabling objects consisting of a tree of nodes with associated properties. It is compliant with the Java Content Repository API and implemented by relying on Apache Jackrabbit for the object structure and node properties. Node content is outsourced to other services. Every data to be managed in a VRE has a manifestation in terms of Information Objects. The unification of the entire data space makes it possible to realise services across the boundaries of specific data typologies. Among these unifying services there is an innovative search engine [21] that makes it possible to seamlessly discover objects in the data space.

Tabular data. The *Tabular Data Manager* offers a comprehensive and flexible working environment for accessing, curating, analysing and publishing tabular data. It enables a user to ingest data – from a file or a web location – that are represented in formats including CSV, JSON and SDMX. In the case of "free" formats, namely CSV, the system offers facilities to transform data in a well-defined table format where the types of the columns are basic data types including temporal and spatial dimensions as well as references to controlled vocabularies, e.g. Code List. Table formats can be defined in an interactive way as well as by relying on templates. Besides constraints on table column types, templates can contain additional validation rules as well as specification of data operations to be performed when an error occurs. Once a tabular data resource is created, it can be manipulated and analysed by benefitting of well known tabular data operations, e.g. adding columns, filtering, grouping, as well as advanced data analytics tasks (cf. Section 2.3). To guarantee a proper and real time management of the data lineage, the service relies on an underlying cluster of RDBMs where any operation on a tabular dataset leads to a new referable version.

Spatial data. gCube owns services realising the facilities of a *Spatial Data Infrastructure* (SDI) by relying on state-of-the-art technologies and standards [22]. It offers standard-based services for data discovery (a catalogue), storage and access (a federation of repositories), and visualisation (a map container). The catalogue service enables the discovery of geospatial data residing in dedicated repositories by relying on GeoNetwork and its indexing facilities. For data storage and access, gCube offers a federation of repositories based on GeoServer and THREDDS technologies. In essence, the infrastructure hosts a number of repositories and a *GIS Publisher Service* that enables a seamless publication of geospatial data while guaranteeing load balancing, failure management and automatic metadata generation. It relies on an open set of back-end technologies for the actual storage and retrieval of the data. Because of this, the GIS Publisher Service is designed with a plug-in-oriented approach where each plug-in interfaces with a given back-end technology. To enlarge the array of supported technologies it is sufficient to develop a dedicated plug-in. Metadata on available data are published by the catalogue. For data visualisation, the infrastructure offers *Geo Explorer* and *GIS Viewer*, two components dedicated to support browsing and visualisation of geospatial data. In particular: Geo Explorer is a web application that allows users to navigate, organise, search and discover layers from the catalogue via the CSW protocol; GIS Viewer is a web application that allows users to interactively explore, manipulate and analyse geospatial data.

Biodiversity data. The *Species Data Discovery and Access Service* (SDDA) [23] provides users with facilities for the management of nomenclature data and species occurrences. As data are stored in authoritative yet heterogeneous information systems, SDDA is mainly conceived to dynamically "aggregate" data from these systems and unify their management. It is designed with a plug-in based architecture. Each plug-in interacts with an information system or database by relying on a standard protocol, e.g. TAPIR, or by interfacing with its proprietary protocol. Plug-ins conform queries and results from the query language as well as data model envisaged by SDDA to the features of a particular database. SDDA promotes a unifying discovery and access mechanism based on the names of the target species, whether the scientific or the common ones. To overcome the potential issues related to taxonomy heterogeneities across diverse data sources, the service supports an automatic query expansion mechanism, i.e. upon request the query is augmented with "similar" species names. Also, queries can be augmented with criteria aiming at explicitly selecting the databases to search in and the spatial and temporal coverage of the data. Discovered data are presented in a homogenised form, e.g. in a typical Darwin Core format.

2.3. Data processing services

In addition to the facilities for managing datasets, VREs offer services for processing them. It is almost impossible to figure out "all" the processing tasks needed by scientists, thus the solution is to have environments where scientists can easily plug and execute their tasks. gCube offers two typologies of engines: one oriented to enact tasks executions at system level, another oriented to enact task execution at user level. Both of them are conceived to rely on a distributed computing infrastructure to execute tasks. A description of these two engines is given below.

System oriented workflow engine. The *Process Execution Engine* (PEng) is a system orchestrating flows of invocations (processes). It builds on principles of data flow processing appropriately expanded in the direction of interoperability [24]. According to this, PEng includes the plan (flow of execution), the operators (executable logic), the transport and control abstraction, the containers (areas of execution), the *state* holders (e.g. storage), the *resource profiles* (definitions of resources characteristics for exploitation in a plan). It allows to distribute jobs on several machines. Each job defines an atomic execution of a more complex process. Relations and hierarchies among the jobs are defined by means of Direct Acyclic Graphs (DAG). DAGs are statically defined according to the Job Description Language (JDL) specifications [25].

Data analytics engine. The *Data Miner* (DM)[5] is conceived to provide end users with an environment to execute computational analysis of datasets through both service provided algorithms and user defined algorithms [26]. At VRE creation time, the DM is configured with respect to the algorithms to be offered in that context. The DM currently supplies more than 200 ready to use algorithm implementations which include real valued features clustering, functions and climate scenarios simulations, niche modelling, model performance evaluation, time series analysis, and analysis

[5] Formerly known as Statistical Manager. In practice, DataMiner results from the re-engineering of the Statistical Manager service.

of marine species and geo-referenced data. New algorithms can easily be integrated, in fact the DM comes with a development framework dedicated to this. A scientist willing to integrate a new algorithm should develop it by implementing some basic Java interface defining algorithm's inputs and outputs. In the case of non-Java algorithms, e.g. R scripts, the framework provides facilities to integrate them [27]. Integrated algorithms can be shared with coworkers by simply making them publicly available. The DM is designed to operate as a federation of DM instances, all sharing the same capabilities in terms of algorithms. Depending on the characteristics of the algorithm and the data, each DM instance executes the algorithm locally or outsources part of it to the underlying infrastructure including gCube workers (cf. Section 2.1). A queue-based messaging system dispatches information about the computation, which includes (*i*) the location of the software containing the algorithm, (*ii*) the subdivision of the input data space, which establishes the portion of the input to assign to each node, (*iii*) the location of the data to be processed, (*iv*) the algorithm parameters. Workers are data and software agnostic, which means that when ready to perform a task, they consume information from the queue and execute the software in a sandbox passing the experimental parameters as input. DM instances and workers share a data space for input and output consisting of a RDBMS, the Storage Manager, and the Home Library (cf. Section 2.2).

2.4. Collaborative services

VREs are easy to use (e.g. requested skills do not exceed the average scientist's ones), have limited adoption costs (e.g. no software to be installed), look like an integrated whole (e.g. the boundaries of the constituents are not perceived), and have an added value with respect to the single constituent's capabilities (e.g. simplify data exchange).

gCube offers its VREs via thin clients, e.g. a plain web browser. All the facilities so far described are made consumable via specific components, i.e. *portlets*, that are web-based user interface constituents conceived to be aggregated, configured and made available by a portal at VREs creation. To complete its offering and provide its users with added value services, gCube equips its VREs with (*i*) a social networking area, (*ii*) a catalogue, and (*iii*) a user management dashboard.

Social networking. gCube offers facilities promoting innovative practices that are compliant with Open Science [28]. Among the services there is a *Home Social* resembling a social network timeline where VRE users as well as applications can post messages, information objects, processing results and files. Such posts can be discussed and favourited (or questioned) by VRE members in a very open way. Every member is also provided with a *Workspace*, i.e. a folder-based virtual "file system" allowing complex information objects, including files, datasets, workflows, and maps. Objects residing in the workspace can pre-exist the VRE or be created during the VRE lifetime, all of them are managed in a simple way (e.g. drag & drop), can be downloaded as well as shared in few clicks.

Catalogue. gCube offers a catalogue-like facility VRE users can rely on to have a flexible and powerful publishing environment to announce, or being informed of, the availability of research artefacts. The publishing platform is based on the CKAN open source technology.[6] This technology has been largely customised and extended to meet the needs arising in gCube application scenarios. One of the major extensions is related to the "data model" to be supported by the platform. CKAN natively supports the notion of *dataset*, i.e. the managed item. Each of such items is characterised by (*i*) a basic set of attributes (e.g. author, title, description), (*ii*) an open-ended set of additional attributes captured by any (key, value) pair, (*iii*) a set of resources forming the payload of the item, and (*iv*) the organisation the dataset belongs to. This model has been extended by adding the notion of publishable "item type" that by using a templating approach enables to characterise the publishable item typologies by carefully defining the additional attributes (with controlled vocabularies and allowed values) characterising them. In addition to that, it is possible to define systematic tagging strategies per item type as well as systematic assignment of items to *groups*, i.e. collections of items defined for discovery and management purposes. This make it possible for every community served by a VRE to carefully define the publishing practices as well as the objects to be published (e.g. datasets, software, services) and how they are expected to be described and managed. The catalogue is equipped with a dedicated portlet allowing to navigate and access the available content (taking into account the access policies of the items and organisations) and supporting search (keyword based and faceted) and browse (by tag, organisation, group, type) facilities.

User management. gCube offers a rich array of portlets organised in a dashboard to enact VRE managers to easily manage the users of a VRE. Management facilities offered includes (*i*) to be provided with an ever updated list of current VRE members with their roles; (*ii*) to easily manage membership, i.e. accept/reject requests for new membership, withdraw membership; (*iii*) to create and manage groups; (*iv*) to assign/revoke roles to members.

3. Related work

Virtual Research Environments, Science Gateways, Virtual Laboratories and other similar terms [7] are used to indicate web-based systems emerged to provide researchers with integrated and user friendly access to data, computing and services of interest for a given investigation that are usually spread across many and diverse data and computing infrastructures. Moreover, they are conceived to enact and promote collaboration among their members for the sake of the investigation.

There are many frameworks that can be used to build such systems. Shahand et al. [9] have identified eleven frameworks explicitly exploited to develop Science Gateway including Apache Airavata, Catania SG Gateway, Globus, HUBzero(+Pegasus), ICAT Job Portal, and WS-PGRADE/gUSE. Such frameworks are quite diverse, e.g. Apache Airavata offers its facilities via an API while the Catania SG Gateway offers its facilities via a GUI and a RESTful API. However, they share certain characteristics that make them operate at a lower level of abstraction with respect to the one of gCube. For data management, these frameworks mainly focus on files while gCube tries to capture an extensive domain offering specific services (cf. Section 2.2). Moreover, such specific services are conceived to make it easy to collect data from/interface with existing data providers thus to make their content available to VRE members. For data processing, the frameworks analysed by Shahand et al. focus on executing jobs while the gCube Data analytics engine (cf. Section 2.3) complements this key yet basic facility with mechanisms enabling scientists to easily plug their methods into an environment transparently relying on distributed computing solutions. Moreover, every single algorithm once successfully integrated is automatically exposed with a RESTful API (OGC Web Processing Service) thus making it possible to invoke it by workflows. Finally, the mechanism gCube offers for the creation of a VRE is unique (cf. Section 2.1). In essence, authorised users can simply create a new VRE via a wizard driving them to produce a characterisation of the needed environment in terms of existing resources. The software (including GUI constituents) and the data needed to satisfy the VRE specification are automatically deployed, no sysadmin intervention is needed.

[6] CKAN is an open-source system conceived to enact the construction of data hubs and data portals http://ckan.org/.

4. Conclusion

This paper provided a comprehensive description of the design principles characterising the gCube software system and the facilities this system offers to enact the operation of an IT infrastructure enabling the development of *Virtual Research Environments*, i.e. ready to use web-based working environments specifically conceived to provide their designated community with the facilities (services, data, capacity) they need. Virtual research environments are expected to be used primarily via a plain web browser. A screenshot of a typical home of the GUI is in Fig. 3 where the user is provided with the list of VREs he/she is member of (right column), some statistics on his/her activity and a direct access to the workspace (left column), access to the catalogue and the messages and discussions occurring (central column). Fig. 4 showcases a typical home page of a VRE with its own specific menu for accessing the facilities it offers. In addition to web GUIs, there are RESTful APIs for accessing and using VRE services in a programmatic way.[7]

The development of a new VRE by gCube is a task usually requiring few ours including the use of the wizard to define the VRE (see Fig. 2), the approval of the specification and the deploy of the components including the portlets. Once the VRE is in place, the VRE managers can customise the GUI (if needed) by reshuffling the portlets across menu and pages, add some content (e.g. in the workspace) and finally start inviting members. This is the ideal scenario based on the assumption that everything needed to create the VRE has been already developed. In case there are pieces of technology to be developed the time and effort needed to develop such technology depends on several factors including their complexity. In some cases, it is a matter of simply exploiting some gCube services. For instance, if a VRE Manager/member is willing to make available to the rest of VRE members his/her own analytics method (already implemented), he/she should just import such a method by relying on the data analytics importing mechanism (cf. Section 2.3). Another example of extension is about the enlargement of the available data sources. A number of mediators have been developed for accessing biodiversity information systems, the one of interest are simply selected at VRE specification time yet new ones can be developed to deal with new sources. Entire web sites can be integrated in a VRE by relying on a specific portlet taking care of embedding the content of the third party web site and invoking the third party website with a security token enabling the web site to get information on the user invoking it. All in all, the patterns governing VRE development are many and diverse. Developing a new component suitable for being integrated in a VRE also depends on the degree of integration expected, they range from a legacy component simply integrated from the GUI perspective with aspects of authentication and authorisation up to fully fledged new gCube components designed to interface with the rest of gCube components.

The experiences made while exploiting gCube to operate the D4Science.org infrastructure somehow demonstrate that the principles governing the VREs delivery and the system openness are key in the modern science settings [29]. The currently supported VREs are available via dedicated portals, some of these VREs are openly available for exploitation and test.[8] Several use cases have been developed by relying on gCube-based VREs, e.g. to estimated the spread of the puffer fish Lagocephalus sceleratus in the Mediterranean Sea due to suitable environmental conditions in this area and favoured by climate change [30]; to develop a bayesian hierarchical approach for the estimation of length?weight relationships in fishes [31]; to develop a global record of fish stocks and fisheries [32]; to develop a workflow where by sharing photos of an object or an environment it is possible to produce a virtual reality scene as a navigable 3D reconstruction that can be shared with other people [33]. Overall, D4Science is currently serving more that thousands of users (more than 7000 in September '18). In the period January–September 2018 the users served by this infrastructure and its VREs performed: a total of 50,127 sessions, with an average of circa 5569 sessions per month; a total of 4,288 social interactions, with an average of circa 476 interactions per month; a total of 150 millions of analytics tasks, with an average of circa 16 millions tasks per month.

[7] More information are available at https://dev.d4science.org/.

[8] The D4Science Gateway http://services.d4science.org/ offers an up to date list of gCube-based Virtual Research Environments.

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[9] https://www.gcube-system.org/credits.

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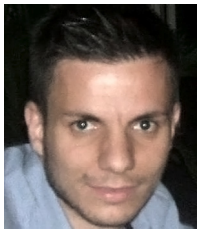

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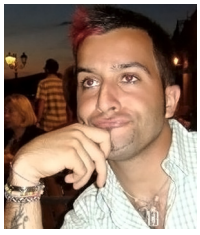

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