VisIVO Science Gateway: a Collaborative Environment for the Astrophysics Community

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Abstract—VisIVO Science Gateway is a web based, workflow enabled environment wrapped around a WS-PGRADE/gUSE portal integrating seamlessly large-scale multi-dimensional astrophysical datasets with applications for processing and visualization based on Distributed Computing Infrastructures (DCIs). We present the main tools and services supported including an application for mobile access to the gateway. We discuss issues in sharing workflows and report our experiences in supporting specialised communities. We present a number of workflows developed recently for visualization and numerical simulations and outline future workflows currently under development. Finally, we summarise our work on the gateway with pointers to future developments.

Keywords—Science Gateways; Workflow Systems; Collaborative Environments; Astrophysics; Large-Scale Datasets; Visualization; DCIs

I. INTRODUCTION

Visualization can play an important role in the context of large-scale multi-dimensional astrophysical datasets, e.g. in understanding, interpreting and verifying their intrinsic characteristics [1]. Often a number of data exploration tools are employed for visual discovery in order to identify regions of interest within which to apply computationally expensive algorithms (e.g. see [2]). Such processes typically involve distributed solutions for storage and processing. Recently science gateways have gained popularity as they allow seamless integration of datasets, tools and applications enabled for executing on generic distributed computing infrastructures (or DCIs).

Science gateways provide services to support searching, managing and uploading/downloading (thus allowing sharing) of applications and datasets. They enable user communities to deploy their applications through common graphical user interfaces, thus allowing scientists to focus on the actual applications instead of learning and managing the required infrastructures. The processes supported by gateways are organized as scientific workflows [3] that explicitly specify dependencies among underlying tasks for orchestrating distributed resources appropriately.

This paper reports on the on-going developments of VisIVO Science Gateway¹ and VisIVO Mobile application, first presented in [4], focusing on some complex case studies to support specialized astrophysics communities (see Section V) which are managed through a workflow sharing framework (see Section IV). Our gateway is wrapped around WS-PGRADE [5], a highly-flexible interface for the grid User Support Environment² (gUSE) and provides access to VisIVO Server tools [6] (see Section II), thus enabling execution of complex workflows through a comprehensive collection of modules for processing and visualization of astrophysical datasets.

A number of customized workflows is configured by default to allow local or remote uploading of datasets, datasets filtering and creation of scientific movies. These workflows are provided with specific user interface portlets to enable intuitive parameter setting for standard users while hiding the complexity of the underlying system and infrastructures. The mobile application employs user accounts from the gateway and offers a handy platform for astrophysical communities to share results and experiences of analysis and exploration of their datasets.

For displaying 2D or 3D plots, astrophysicists typically deploy software packages programs such as Gnuplot, Super-Mongo, or scripting languages such as Python, Matlab or IDL. VisIt³ or ParaView⁴ offer a combination of 2D and 3D plotting capabilities, real-time and offline analysis, scripting and graphical control. VisIt has been provided with grid services for scientific collaborative visualization in UNICORE Grids [7]. ParaView has been extended to offer grid services [8] and a plugin has been developed to provide interactive remote visualization for collaborative environments based on video streams [9].

Nevertheless scientific visualization can be a fairly complex process involving several steps, e.g. filtering data, choosing a representation and desired level of interactivity and customizing the manner in which the data is displayed. None of the aforementioned tools are provided with a science gateway to interface them with workflow services. Within VisIVO Science Gateway and VisIVO Mobile ready to-use workflows can be downloaded, parametrized and executed under a controlled

¹http://visivo.oact.inaf.it:8080

²http://www.guse.hu

³https://wci.llnl.gov/codes/visit

⁴http://www.paraview.org

environment. The visualization and filtering parameters can be chosen interactively and the workflow configuration and submission to DCIs is performed without exposing technical details so that end users can focus on their applications instead of devoting efforts in learning and managing the underlying infrastructures.

II. VISUALIZATION TOOLS

VisIVO [6] is an integrated suite of tools and services for effective visual discovery within large-scale astrophysical datasets. VisIVO is realised as:

- VisIVO Desktop [10], a stand alone application for interactive visualizations running on standard PCs;
- VisIVO Server, a grid-enabled high performance visualization platform, and
- VisIVO Library [11] developed specifically to port VisIVO Server on gLite middleware⁵.

Users of each realization can obtain meaningful visualizations rapidly while preserving full and intuitive control of relevant visualization parameters. This section focuses on VisIVO Server⁶ which can be installed on any web server with a database repository and contains the following distinct modules: VisIVO Importer, VisIVO Filters and VisIVO Viewer (see Figure 1).

VisIVO Importer converts user-supplied datasets into VisIVO Binary Tables (VBTs). A VBT is a highly-efficient data representation realized through a header file containing all necessary metadata and a raw data file storing actual data values. VisIVO Importer supports conversion from several popular formats such as: ASCII and CSV, VOTables or FITS Tables without imposing any limits on sizes or dimensionality. VisIVO Filters is a collection of data processing modules to modify a VBT or to create a new VBT from existing VBTs. The filters support a range of operations such as scalar distribution, mathematical operations or selections of regions. VisIVO Viewer is the visualization core component based on the Visualization ToolKit7. It creates 3D images from multi-dimensional datasets rendering points, volumes and isosurfaces. Moreover there is support for customized look up tables and visualizations using a variety of glyphs, such as cubes, spheres or cones. VisIVO Viewer can be also used to produce images in a given sequence of azimuth, elevation, and zooming values that can be externally mounted to produce movies.

To create customized renderings from astrophysical data tables VisIVO Importer is first utilized to convert user datasets into VBTs. Then, one or more VisIVO Filters can be applied to process these datasets, and finally VisIVO Viewer is invoked to display these renderings. Figure 1 illustrates the typical sequence of steps required within the VisIVO Server processing pipeline.

⁵http://glite.cern.ch

⁷http://www.vtk.org





III. VISIVO SCIENCE GATEWAY AND VISIVO MOBILE Application

The existing VisIVO Web [12] has been integrated within the WS-PGRADE/gUSE generic gateway [13] to offer new, easily accessible opportunities not only to scientific users, e.g. astrophysical researchers, but also to the wider public, e.g. high-school education or innovative citizen science activities. This work is supported by the SCI-BUS project⁸ providing operation and maintenance of the gateway as well as endusers support for training activities. A special focus of the work has been placed on standardization and quality control issues in order to increase the chances of adoption (by other relevant user communities) of the developed technologies and methodologies.

A. VisIVO Science Gateway Main Services

The VisIVO Science Gateway is designed as a workflow enabled grid portal that is wrapped around WS-PGRADE providing visualization and data management services to the scientific community by means of an easy-to-use graphical environment for accessing the full functionality of VisIVO Server. Complex workflows can be created and executed on a variety of infrastructures (e.g. clouds, desktop and service grids or supercomputers) to obtain comprehensive exploration and analysis of large-scale astrophysical datasets. The gateway offers role-based authorization modules and supports secure login.

Currently a number of main roles are implemented for access as follows: guests, standard and advanced users and administrators [4]. Standard users can upload and manage their datasets through portlets without any knowledge about the (conveniently hidden) underlying grid-infrastructure and middleware. By using interactive widgets users can construct customized renderings, or store data analysis and visualization results for future reference. Their datasets are managed internally through a relational database preserving their metadata and maintaining data consistency. Figure 2 shows the main portlets of the Gateway connecting to VisIVO Importer, Filters and Viewer services.

Both remote and local datasets can be uploaded - i.e. residing on a remote URL or locally on a user's PC. For

⁶http://sourceforge.net/projects/visivoserver

⁸http://www.sci-bus.eu



remote files the user must specify URL and optionally a user name and password for authentication. Depending upon the size of the datasets under consideration, remote uploads could last a long period. To resolve this situation VisIVO Gateway allows an off-line mode by means of a workflow submission so that users can issue upload commands and then simply close their current session - a follow up e-mail typically gives notification once the uploading operation is completed. The workflow employed for remote importing is illustrated in Figure 3. It allows generation of significant information for meta data exploration, e.g. statistics on data values, histogram calculation and plotting or a sample extraction of uploaded datasets. Such meta data is available through the Properties portlet and some can be modified by the user (e.g. renaming VBTs or related fields).



VisIVO Gateway automatically displays all applicable VisIVO Filter operations allowing input of the relevant parameters. Finally the VisIVO Viewer is employed for image display. A right click on any processed dataset in the Data Management portlet is used in conjunction with the View button to create user-prescribed VisIVO Viewer views. VisIVO Gateway further allows users to generate scientific movies. These can be useful not only to scientists to present and communicate their research results, but also to museums and science centres to introduce complex scientific concepts to general public audiences.

Users can create a *Panoramic Movie* by moving a camera along a motion path of 360° in azimuth and $+/-90^{\circ}$ in elevation within the dataset's domain. *Customized Movies* can be produced by intermediate snapshots specified as camera positions/orientations and the gateway generates a movie with a camera path containing these specified positions/orientations. *Dynamic Movies* can be created by interpolating several steps of a time evolution of a cosmological dataset. The user can browse a cosmological time evolution and choose two or more coherent datasets. The designed workflow will then produce the necessary number of intermediate VBTs by calculating particle positions and applying boundary conditions as necessary. This approach can be very useful, e.g. in revealing galaxy formation or observing large-scale structures such as galaxy clusters.

The creation of a movie represents a significant challenge for the underlying computational resources as often hundreds or thousands of high quality images must be produced. For this reason Parameter Sweep (PS) workflows [14] are employed. This is particularly relevant to the visualization-oriented workflows presented in Section V. As the respective communities typically employ a large number of parameters that have to be varied within user-defined ranges, several hundreds to thousands of workflow executions might be necessary. As an example a panoramic movie is generated with the workflow shown in Figure 4, it generates four movies with different camera position paths on the generator port: from 0° to 360° azimuth rotation, from 0° to 90° elevation rotation, from 90° to -90° elevation rotation and from -90° to 0° elevation rotation. The generation of these four movies is executed in parallel and is finally merged through a collector port as shown in Fig. 4.



B. VisIVO Mobile Application

Once the data file is uploaded a sequence of simple actions is required to rapidly obtain meaningful visualizations. Typically various VisIVO Filter operations are performed, and The VisIVO Mobile application (see Fig. 5) allows smartphone devices to exploit VisIVO Gateway functionalities to access large-scale astrophysical datasets residing on a server repository for analysis and visual discovery. Through interactive widgets, customized visualizations (images or movies) can be generated and stored on the remote server. The application notifies users when requested visualizations are available for retrieving on their smartphones and allows sharing of data, images and movies via e-mail or by exploiting common social networks.

Fig. 5. VisIVO Mobile screenshots on an iPad device: navigation through the imported datasets and produced images and scientific movies (upper figure); and dataset remote importing (lower figure).



The current version of VisIVO Mobile is implemented in Objective-C optimized for the Apple iPhone, iPod and iPad, and, in the near future, it will be ported to other popular smartphone devices. End users can login with the same credentials as on the gateway and the application provides the password coding in SHA cryptography exploiting the built-in functionalities of the Liferay⁹ environment and querying the remote database to verify access credentials. The configuration and submission of workflows residing on the VisIVO Gateway is performed by means of the gUSE Remote API [13]. This API interfaces to the core gUSE services without the WS-PGRADE user interface component. Thus running and managing scientific workflows is realized by command line solutions consisting of curl¹⁰ based access wrapped in shell scripts. The API exposes usage of gUSE components through a simple web service interface, resulting in wide adaptability by a diverse set of tools and programming languages.

⁹http://www.liferay.com

C. Implementation Details and Computing Infrastructures

The VisIVO Science Gateway is based on the collaborative and community oriented application development environment WS-PGRADE/gUSE. There is full integration in the portal framework Liferay which is highly customizable thanks to the adoption of portlet technology defined in the Java Specification Request 168 and 286¹¹, and compatible to modern web applications. The implemented portlets are developed with the Java Vaadin web Framework¹². This open source framework has been employed to implement server side Java Servlet based web applications using the full power and flexibility of Java without taking care of the client side since it compiles the Java source code to JavaScript which can then be run on any browser.

The current architecture of VisIVO Science Gateway has a distributed configuration on different machines enhancing the service performances as shown in Figure 6. The front-end services contain WS-PGRADE and Liferay and the back-end services include the gUSE components. The database server resides on the back-end machine. The VisIVO community of advanced users are enabled to create, change, invoke, and monitor workflows accessing to all of the components of WS-PGRADE/gUSE, while standard users are provided with the easy-to-use specific web based user interfaces described in Section III-A including the gUSE Application Specific Module (ASM) API [15] to reuse the implemented workflows stored in the local repository of gUSE. The VisIVO Mobile application configures and submits workflows residing on the VisIVO Gateway by means of the gUSE Remote API as described in section III-B.





The VisIVO Science Gateway currently exploits the Cometa Consortium grid¹³. This infrastructure is distributed in

¹⁰http://curl.haxx.se/

¹¹http://jcp.org/en/jsr

¹²http://www.vaadin.com

¹³ http://www.consorzio-cometa.it

seven sites of Sicily. All sites have the same hardware and software configuration allowing high interoperability and realizing an homogeneous environment. The computing infrastructure is based on IBM Blade Centre each containing up to 14 IBM LS21 blades interconnected with the low latency Infiniband-4X network, to provide High Performance Computing (HPC) functionalities on the grid. There are currently about 2000 CPU cores and more than 200 TBs of disk storage space available on this HPC e-Infrastructure. As reported in [4] the VisIVO Science Gateway is undergoing testing under the ETICS system [16] based on the Metronome software [17] by 4D Soft¹⁴. Web testing has been adopted by 4D Soft mainly because it is platform and application independent for testing in different environments and supports different technologies in a uniform way through test libraries. Currently a number of tests is under development suitable for the VisIVO Mobile application.

IV. SHARING WORKFLOWS

Building large workflows from scratch to address scientific communities can be time-consuming, as it is inherently a multi-disciplinary process. As an example, although astrophysicists might be able to appreciate the benefit to their work in using a workflow, they are less interested in the technical details for developing it, this is a task that is naturally associated with the developers (typically computer scientists). Manually monitoring the evolving structure of workflows, e.g. by email or written documentation, can be quite challenging. The plan is then to not only educate non computer science scientific communities in using workflows, but to also provide them with high level tools so that they can access the results of these workflows intuitively. Effective collaboration requires ways to facilitate exchange between different groups, in particular enabling sharing and realizing re-use and interoperability. The SHIWA project¹⁵ (SHaring Interoperable Workflows for large-scale scientific simulations on Available DCIs) provided solutions to facilitate sharing and exchanging of workflows between workflow systems and DCI resources through the SHIWA Simulation Platform (SSP) consisting of:

- SHIWA Repository¹⁶: A database where workflows and meta-data about workflows can be stored. The database is a central repository for users to discover and share workflows within and across their communities.
- SHIWA Portal¹⁷: A web portal that is integrated with the SHIWA Repository and includes a workflow executor engine that can orchestrate various types of workflows on a number of computational grid/cloud platforms.

Through the SHIWA Portal one can define and run simulations on the SHIWA Virtual Organisation which is an einfrastructure that gathers computing and data resources from various DCIs, including the European Grid Infrastructure. The portal (via third party workflow engines) provides support for a number of commonly used academic workflow engines and it can be extended with other engines on demand. Such extensions translate between workflow languages and facilitate the nesting of workflows into larger workflows even when those are written in different languages and require different interpreters for execution. This functionality can enable scientific collaborations to share and offer workflows for reuse and execution. Shared workflows can be executed on-line, without installing any special client environment for downloading workflows.

V. SUPPORTING COMMUNITIES

A number of challenging workflows has been prototyped recently to support highly specialised scientific communities mainly in astrophysics. This section discusses our experiences with the visualisation-oriented workflows *Muon Portal* and *LasMOG*, and the simulation-oriented workflow *FRANEC*. The former are deployed for detecting nuclear threat materials (see V-A) and investigating large-scale modified gravity models (see V-B) respectively. The latter is exploited for carrying out stellar evolution simulations. These workflows will be supported in ER-flow¹⁸ so that they can be stored into the SHIWA workflow repository together with related meta-data, allowing investigation of their interoperability and dissemination across relevant communities through the SHIWA simulation platform.

Advanced users can exploit such workflows as templates for building new customized workflows to suit particular requirements of scientific communities, e.g. by modifying appropriately constituent building blocks customized *LasMOG* workflows can be generated. Standard users can then execute these workflows in an interactive and user-friendly way by means of the supplied portlets. Any user can submit jobs to the underlying DCIs without requiring a priori any specific technical expertise related to the particulars of the DCI configuration.

We are currently in the planning stages of developing a number of new visualisation-oriented workflows to be deployed for rapid discovery of supernova light curve anomalies¹⁹ and validation of models reconstructing the large scale structure of the universe²⁰²¹. Furthermore two simulationoriented workflows are under development, the first one will be deployed for studying trajectories of interstellar comets passing through the Solar System and the second one will be focused on modelling the dynamical evolution of meteoroid streams. The vision is that, once a sufficient number of visualisation-oriented and simulation-oriented workflows has been developed, to analyse any similarities in depth towards developing templates for generating classes of workflows to address the needs of specialized scientific communities. The remaining of this section focuses on the *Muon Portal, LasMOG* and *FRANEC* workflows.

A. Muon Portal

The deflection of muonic particles present in the secondary cosmic radiation results from crossing high atomic number materials (such as uranium or other fissile materials). This can

¹⁴http://etics3.4dsoft.hu

¹⁵ http://www.shiwa-workflow.eu

¹⁶http://shiwa-repo.cpc.wmin.ac.uk

¹⁷http://shiwa-portal2.cpc.wmin.ac.uk/liferay-portal-6.1.0

¹⁸ http://www.erflow.eu

¹⁹http://supernovae.in2p3.fr/~guy/salt

²⁰http://www.mpa-garching.mpg.de/gadget

²¹https://github.com/cmcbride/bgc_utils

significantly improve on the success rate of current nuclear threat detection methods which are based on X-ray scanners [18], especially in terms of capacity for identification and location of illicit materials inside cargo containers, even considering the possibility of screens designed to mask their existence [19].

We have developed a visualisation-oriented workflow suitable for inspection of cargo containers carrying high atomic number materials, by displaying tomographic images [20]. Preliminary results of this workflow have been reported in [4]. The datasets containing coordinates of the muon tracker planes are first uploaded to our gateway and filtered by using the Point of Closest Approach (POCA) algorithm [21] to create a representation containing the scattering deflection of cosmic radiations. The result is then visualized using point rendering.

Further processing is then applied based on user-defined thresholds, followed by conversion into data volumes using the deflection angle field distribution by employing the 3D Cloudin-Cell (CIC) [22] smoothing algorithm. Finally, a tomography is performed for inspection. Figure 7 shows the most recent development and results of the entire computational process starting from: a) parameter setting through the supplied portlet, then b) submitting the implemented workflow, and finally c) outputting resulting images obtained using isosurface rendering for the filtered (top image) and raw (bottom image) datasets respectively.

Fig. 7. Muon Portal processing: portlet interface, workflow and selected results.



B. LasMOG

The acceleration of the Universe is one of the most challenging problems in cosmology. In the framework of general relativity (GR), the acceleration originates from dark energy. However, to explain the current acceleration of the Universe, the required value of dark energy must be incredibly small. Recently efforts have been made to construct models for modified gravity (i.e. without introducing dark energy) as an alternative to dark energy models [23].

Observing the large scale structure of the universe could in principle provide new test of GR on cosmic scales. This kind of test cannot be done without the help of simulations as the structure formation process is highly non-linear. Largescale simulations are thus performed for modified gravity models, e.g. from the Large Simulation for Modified Gravity (LaSMoG) consortium.

Fig. 8. LasMOG processing: portlet interface, workflow and selected results.



The workflow shown in Figure 8 implements a customised visualization for aiding analysis of modified GR simulations, more specifically inspecting datasets to discover anomalies by comparing appropriately with datasets coming from standard GR models. The main computational steps are summarised as follows:

- Two datasets corresponding to snapshots of standard gravity (*D_S*) and modified gravity (*D_M*) model simulations are processed.
- Sub-samples of the point distributions with a reduced number of points in the two datasets are generated. Then, for each of these sub-samples a panoramic movie is created (as shown in the resulting top image of Figure 8).
- A point distribute operation is performed on D_S and D_M to create new volume datasets (V_S and V_M respectively) using a field distribution algorithm on a regular mesh.
- A volume property on the same computational domain is distributed on a regular mesh producing a density field.
- A new volume V_∆ is computed where each of its voxels shows a difference of values in the density between V_S and V_M. It is then filtered with a lower bound threshold and all the voxels satisfying the filters

are saved in a text file for further analysis purposes (as shown in the resulting bottom image of Figure 8).

- Several renderings of V_{Δ} are performed:
 - Volume rendering;
 - Isosurface rendering of the density field to produce panoramic movies using different isovalues (as shown in the resulting bottom image of Figure 8);
 - Ortho-slice rendering i.e. orthogonal slice planes through the volume dataset.

C. FRANEC

FRANEC is a state-of-the-art [24] numerical code for stellar astrophysics. This code is perfectly suited for computing evolutions of stars on the basis of a number of different physical inputs and parameters. A single run of FRANEC produces one synthetic model (SM). To produce an isochrone, for a given chemical composition, through a FIR (Full Isochrone Run), it is necessary to execute a large number of SMRs (SM runs) varying the initial mass of the stellar models. Once these evolutionary tracks and isochrones (and other additional data) are computed, they can be distributed in datasets over different sites.

The simulations of stellar models produce simulation output files with a set of associated metadata. Such metadata are linked to all parameters concerning the numerical evolutionary code. In this way it is possible to store and easily search and retrieve the obtained data by many sets of stellar simulations, and furthermore get access to a large amount of homogeneous data such as tracks and isochrones computed by using FRANEC. The FRANEC workflow (see Figure 9) has a modular architecture making it easy to identify reusable modules for building other workflows. Modules can be differentiated on the basis of their functionality:

- 1) *EOS Computation* module provides the Equation of State in tabular form. The input values are the Metallicity Z and the type of mixture (combination of chemical elements heavier than helium).
- 2) *OPACITY Computation* module produces a table of Opacity from pre-calculated tables. Given the Metallicity value Z and the type of mixture it obtains a new table of opacity which is interpolated from the pre-calculated ones.
- 3) FRANEC is the core module of the workflow. It produces the models of stellar evolution starting from the output of the two modules EOS and OPACITY and a set of input parameters given by the user to perform the evolution: the mass (in Solar Units) of the structure, the mass fraction of the initial helium, the mass fraction of the heavy elements abundance, the efficiency of superadibatic convection, the mass loss, the core convective overshooting during the Hburning phase, the diffusion index and the evolutionary stage index . It produces a set of parameter values varying in relation to time, quantities varying in relation to the radius of the model, the chemical composition of the core (vs. time), surface chemicals (vs. time), and energy resolution flows(vs. time).

Fig. 9. FRANEC processing: portlet interface, workflow and selected results.



- 4) *Output Post-Processing* module consists of the following jobs:
 - *TAR* produces a compressed archive of the main outputs.
 - *GNUPLOT* produces the output plots (e.g. the ones included in Figure 9).

VI. CONCLUSIONS

Traditionally the common practice among astronomers for data exploration tools was to employ small, individually created and executed applications. This scenario is not applicable to modern large-scale datasets. Modular web applications for data analysis and visual discovery making effective usage of modern e-infrastructures can be instrumental in reaching out astrophysical communities and aiding them in new scientific discoveries.

A workflow-oriented gateway allows scientists to share their analysis workflows and identify best practices for investigating their datasets. More importantly, they can automate workflows for repeated analysis with changed parameters, which in the past was a manual, slow and very error prone process. This way scientists can focus on core scientific discoveries rather than wasting time on data analysis on dealing with inadequate resources.

VisIVO Gateway provides a web based portal for setting up, running and evaluating visualizations in astrophysics for large-scale datasets exploiting DCIs resources. The gateway includes a data repository containing images and movies produced from imported datasets, as well as repositories of fundamental workflows, which can be used as templates for generating new workflows to be distributed by the users of the system.

We presented several portlets running in a Liferay portal environment together with a mobile application making the gateway accessible from modern mobile platforms. For a number of specialised astrophysical communities we have discussed workflows and the issues involved in developing them. The modularity achieved by subdividing workflows into a number of core tasks ensures re-usability and provides high flexibility. End users do not need to be aware of set-up options or be aware of the computing infrastructure operating behind the scenes.

We envisage building a specialized repository of astrophysics workflows core modules to share them among communities using the SHIWA platform. Our vision for these is to be used not only by astrophysical communities but to also be potentially exploited within other scientific contexts. This activity will also be instrumental in future work for creating an Astro-Gateway Federation establishing a network of Science Gateways to benefit astrophysical communities sharing tools and services, data, repositories, workflows and computing infrastructures.

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