GCS: BioCompute Object Genomics Compliance Suite User Manual

October 2019

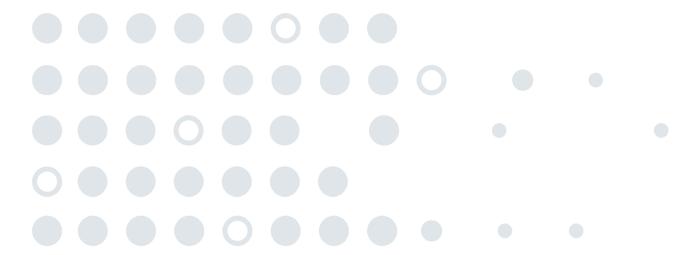


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Goals

Hello, and welcome to the Genomics Compliance Suite (GCS). This manual walks through several steps involved in BioCompute object (BCO) file generation in the GCS. The app guides a user for the generation of BCO manually, or by first selecting bioinformatics workflows written in the Common Workflow Language (CWL), and then by allowing the user to enter text for BioCompute fields described in the BioCompute specification.

Briefly, the goals of this user manual are:

- Learn about the application
- Fetch the CWL workflows in your project, identify and manipulate to generate BCO files
- Download the generated BCO JSON file
- Generate PDF reports for the generated BCO file
- Upload generated BCO file to any of the Seven Bridges platforms or your GitHub account

Getting Started with the Genomics Compliance Suite (GCS)

App Access and Login

The GCS app is designed to be easily deployed locally for testing or on any remote servers for production. A Dockerized version is available on GitHub. Seven Bridges employees can access the app from the internal portal. We are also testing access with academic groups through the Cancer Genomics Cloud.

Dockerized app

Pull or build the Docker image from GitHub (see REAME.md) for details. Run the Docker container. Go to the app served by the Docker container at http://127.0.0.1:3838 in your web browser, and login with the default username and password sevenbridges/sevenbridges (Figure 1).

Seven Bridges hosted app

If you are logging on within Seven Bridges, the following instructions are pertinent to those logging on from within the Seven Bridges VPN.

Go to the hosted version https://shiny-internal.sbgenomics.com/gcs/ (behind the VPN) and log in with your username and password.

RStudio Server on the Cancer Genomics Cloud

Getting the app

Copy the 'biocompute-composer.zip' to your project folder. Please request access to the zip file if you do not currently have access.

Running the app

To run the app:

- Click "Interactive Analysis", then open "Data Cruncher".
- Click "Create your first analysis", select "RStudio" and start the analysis.
- When the editor is launched, switch to the "Terminal" tab in the lower left panel, run the following commands to copy the app from the project to the analysis session:

```
cp /sbgenomics/project-files/biocompute-composer.zip /sbgenomics/workspace/
unzip -q /sbgenomics/workspace/biocompute-composer.zip
rm /sbgenomics/workspace/biocompute-composer.zip
```

- Go to the biocompute-composer folder in the files panel (lower right), open and run through the code in app-setup.R to setup the environment (use Ctrl + Enter to run the code line-by-line).
- Open app.R, click the "Run App" button in the code editor panel to run the app.
- A dialog about popup windows may appear if you're running this for the first time, click "Try Again" to proceed.
- Note: if running the app from a restarted analysis session, remember to run app-setup.R again before running the app.

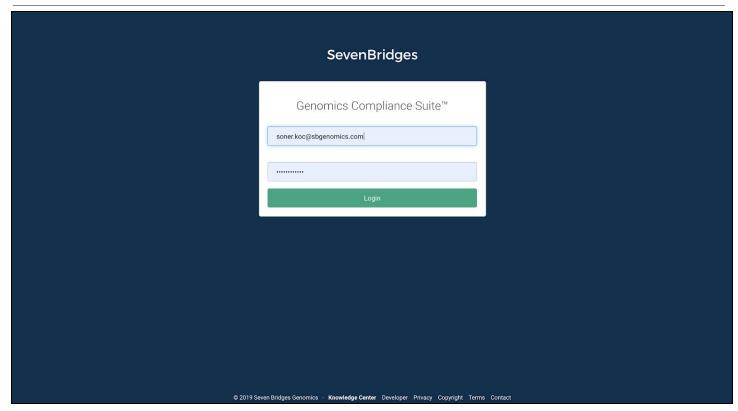


Figure 1: Login Page of the Genomics Compliance Suite

Start Page

You will see the welcome page of the GCS app after your first login:

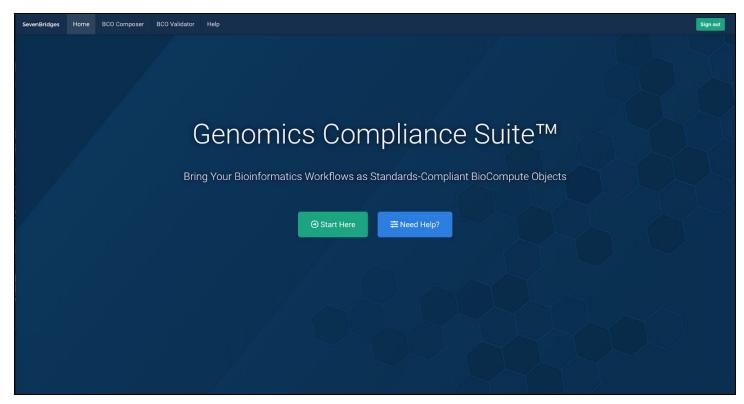


Figure 2: Welcome Page of the Genomics Compliance Suite

In the middle of all, you see the quick action buttons; you can quickly start to build your BioCompute (BCO) object file with "Start Here" button, or you can access the informative page about the BCO with "Need Help?" button.

In the navigation bar, you will see the list of tabs for the main features, such as **BCO Composer (manual mode)**, **BCO Composer (from CWL)**, **BCO Validation, Interactive BCO Browser**, and **Help**.

To save us some time, we will walk through the BCO Composer (from CWL) feature below in detail. All the other features should follow the same principles and are intuitive to use.

BioCompute Object (BCO) Composer

Step 1 - Import the Target CWL App

After you click the "**BCO Composer**" page of the GCS platform, you will see the initial step of the BCO generation, import step (Figure 3).

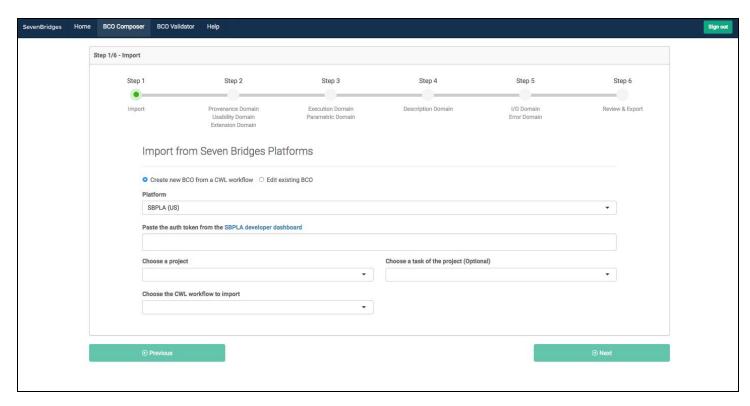


Figure 3: Initial Page of the BCO Composer

The BCO Creator/Composer has six different steps to generate a new BioCompute Object (BCO) to cover each of the BCO domains from the ground up (Figure 4).

It begins with Common Workflow Language (CWL) importing step then goes with Step 2, which has information about Provenance, Usability, and Extension Domains. In Step 3, you can see the Execution Domain and Parametric Domain fields of a BCO sample. Then it goes with Step 4 that has Description Domain. Step 5 follows with I/O Domain and Error Domain. In the end, the user can review the generated BCO and take action like download the BCO file, upload it to your Seven Bridges platform accounts or GitHub accounts.

The "Import" step collects some information from a user to initiate the generation process. These are: **Platform**, **Authentication Token**, **Project**, **Task of the Project** as an optional, and **Application Name** to import the CWL of the selected application.



Figure 4: Steps of the BCO Composer

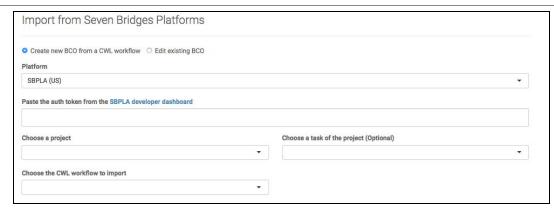


Figure 5: Necessary information fields at the beginning of the BCO Composer

Select a name for a "Platform" that you want to fetch a CWL file of an application (Figure 5).

After that, paste your authentication token to "Paste the auth token from ..." field. Colored text in the name of the field is a direct link to the authentication token page of the selected platform (Please check **Appendix I** to learn more about how to generate authentication token).

When the authentication token of the user is pasted, projects, tasks, and applications that exist in the account of the user will be fetched.

User can select a project to focus on in "Choose a project" field. Then, a task can be selected among the existing tasks in the selected project from "Choose a task of the project" field, which is optional.

Finally, the target application can be selected from "Choose the CWL workflow to import" field to fetch a CWL of a target application to work with to generate a BioCompute Object.

Filled entries of the page are illustrated in Figure 6 and Figure 7.

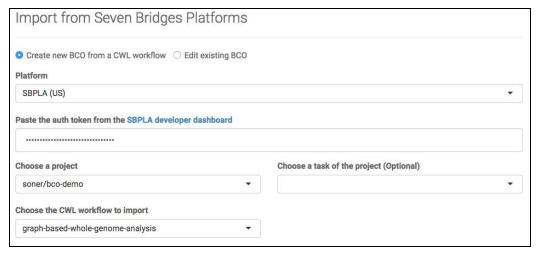


Figure 6: Illustration of the necessary information fields

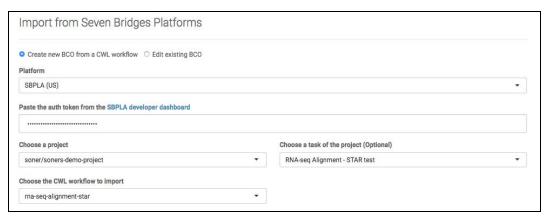


Figure 7: Illustration of the necessary information fields with the optional (task) selection

Step 2 - Provenance, Usability, and Extension Domains

In step 2, Provenance, Usability, and Extension Domains of BCO are listed with their identification fields.

After selecting the target application's CWL file, the GCS app fetches and parses the selected CWL in the background to pre-fill standard information fields between CWL and BCO fields. It is illustrated in Figure 8. On the other hand, some of the fields of BCO cannot be filled by the information parsed from CWL, as shown in Figure 9. Users can add new information into these fields manually. Users can also edit the pre-filled fields according to their needs.

You can find the complete detailed list of Provenance, Usability, and Extension Domain fields in Appendix II, Table 2, and Table 4.



Figure 8: Filled fields, by CWL of the selected application, of domains exist in Step 2



Figure 9: Unfilled fields, by CWL of the selected application, of domains exist in Step 2

Step 3 - Execution and Parametric Domains

In step 3, Execution and Parametric Domains of BCO are listed with their identification fields.

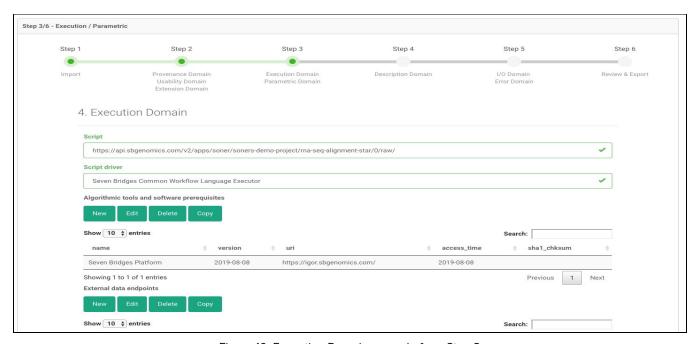
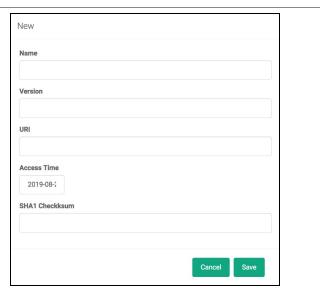


Figure 10: Execution Domain example from Step 3



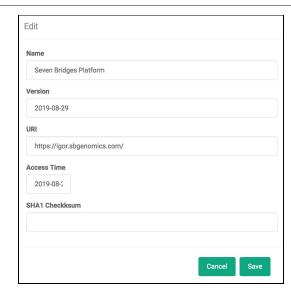


Figure 11: Example of adding a new entry or editing existence one in the field

You can find the complete detailed list of Execution and Parametric Domains' fields in Appendix II, Table 6, and Table 7.

Step 4 - Description Domain

In this step, Description Domain of BCO is listed with its identification fields.

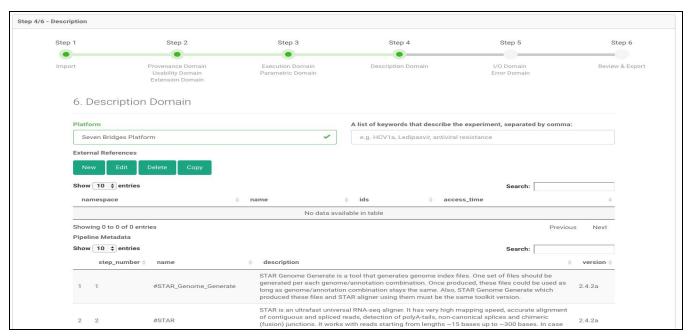


Figure 12: Description Domain example from Step 4

You can find the complete list of the details of the Description Domain fields in Appendix II and Table 5.

Step 5 - I/O and Error Domain

In step 5, Input/Output and Error Domains of BCO is listed with their identification fields.

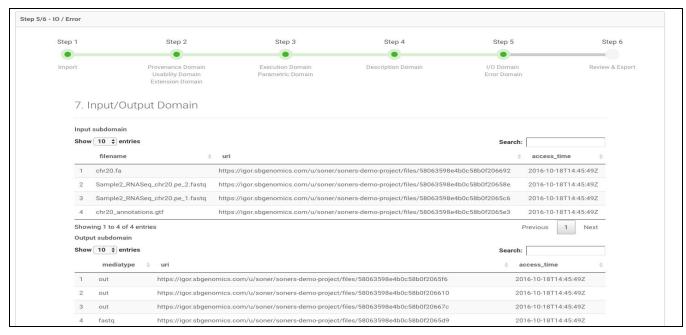


Figure 13: I/O Domain example from Step 5

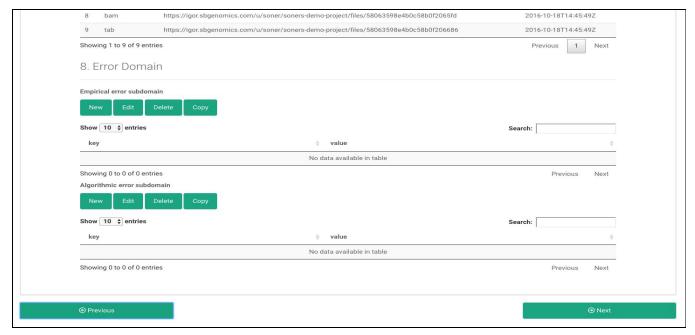


Figure 14: Error Domain example from Step 5

You can find the complete detailed list of I/O and Error Domains' fields in Appendix II, Table 8, and Table 9.

Step 6 - Review and Export

As the last step of BCO Composer, you can review your generated BCO file in "Review & Export" after "Generate & Preview BCO" button is clicked. At the top of them, the "BCO ID" of the generated BCO file is automatically assigned.

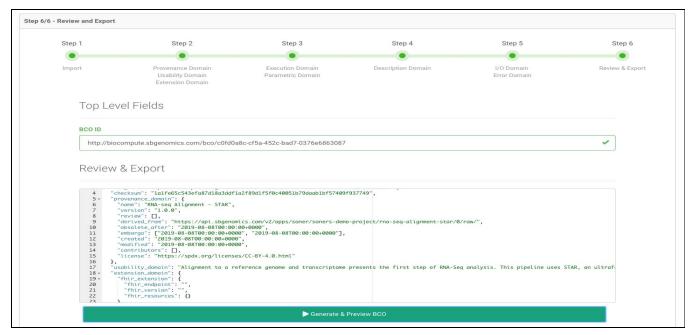


Figure 15: Review the generated BCO file

At the bottom of the review part, users can access some export and save features (Figure 16). The first one is the feature to export the generated BCO file in JSON file format, "**Export as JSON**". When it is clicked, the generated BCO file is downloaded as a JSON file. You can see the example of the exported file in Figure 17.

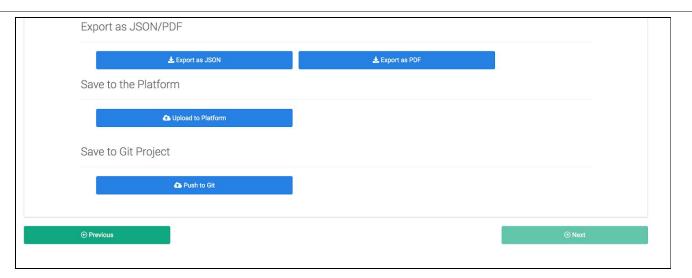


Figure 16: Export and Save Features in Step 6

Figure 17: Example View of the Downloaded BCO JSON file

As the second feature, users can generate a PDF reports for the BioCompute Object with "**Export as PDF**" button. In the report, users can find all domains of the generated BCO file, BioCompute Object specifications, and typed raw JSON of the generated BCO, with white spaces for reviewers to review (Figure 18).

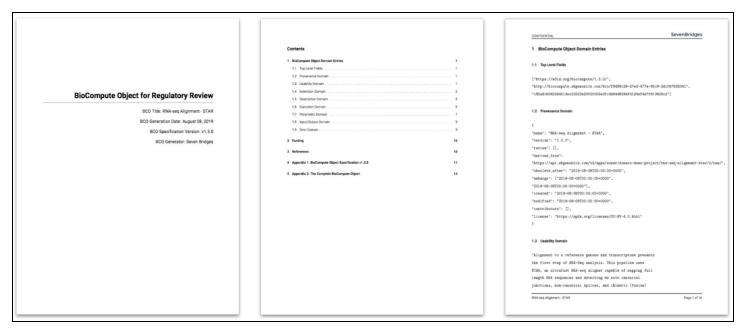


Figure 18: Example View of the Generated PDF Report in Step 6

In addition to export features, there are two very useful save features in the Genomics Compliance Suite: **Save to the Platform** and **Save to GitHub**.

The first one is **Save to the Platform**, automatically saves the generated BCO file into "**BCO**" folder under "**Files**" of your project. You can see the example of the generated files in the project's "**Files/BCO**" folder in Figure 19. Also, there is no need to open the platform in the external browser window. When "**Save to the Platform**" button is clicked, the direct link button (to the platform) appears near the "**Save to the Platform**" button to access the generated file on the platform easily (Figure 20).



Figure 19: Generated BCO Exported to the Platform



Figure 20: Save to the Platform with Direct Link to the Platform in Step 6

As a second, **Save to GitHub**, automatically saves the generated BCO file into your Github account to make your projects up to date and easy-to-access to your BCO files. You can see the **GitHub Connection** popup window, when your click the **Push to GitHub** button (Figure 21).

The window will need the **username** and **password** of the user's GitHub account to make the connection and push operations. Then, the user can type the target **Repository Name** to push the generated BCO file. Also, there is the **Git Commit Message** field that is the explanatory message for the push operation. In the end, when the user clicks on **Push**, results of the push operation will be listed in **Git commit message** area (Figure 22).

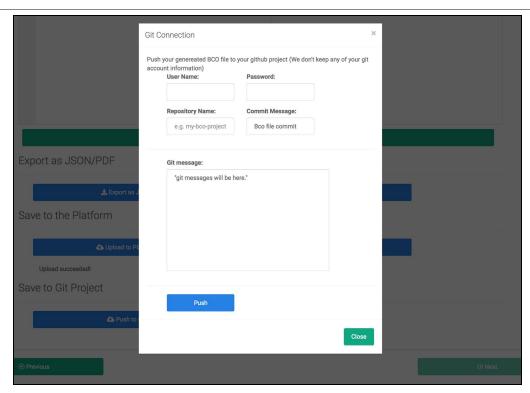
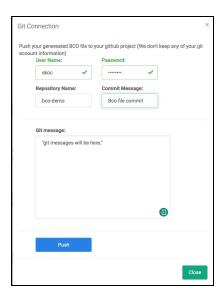


Figure 21: Git Connection Window in Step 6



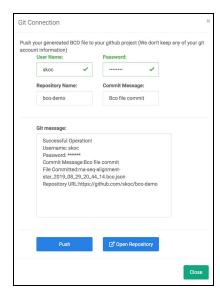


Figure 22: Git Connection Before/After Push Operation in Step 6

BioCompute Object (BCO) Validator

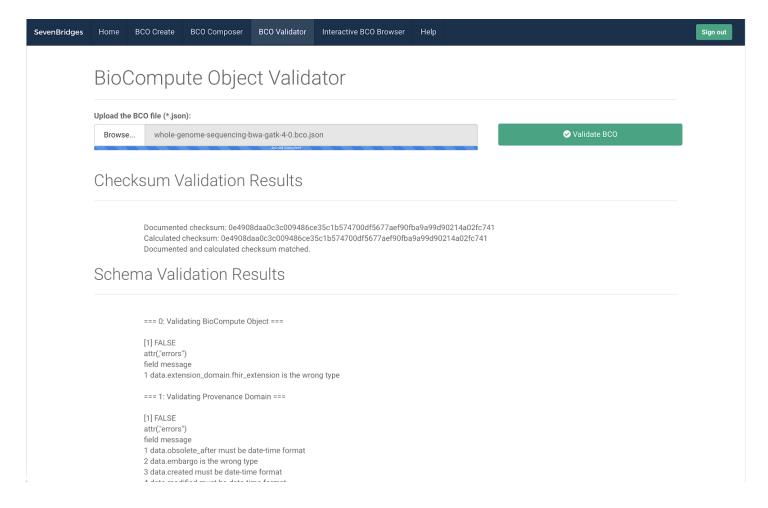


Figure 23: A screenshot of the BCO validator UI.

Interactive BCO Browser

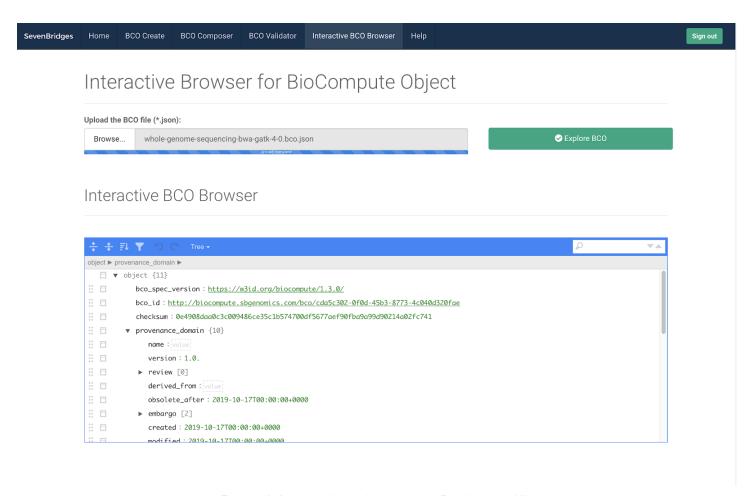


Figure 24: A screenshot of the interactive BCO browser UI.

Appendix I: Platform Authentication Guide

Authentication Token

Your authentication token encodes your Seven Bridges Platform credentials and uniquely identifies you on the Seven Bridges Platform. It can be used with a number of API and automation features of the Seven Bridges Platform without the need of a manual, GUI authentication process.

Locate Authentication Token

You can get your authentication token from the developer dashboard. For example, for Seven Bridges Platform users, click <u>here</u> to go to the developer dashboard to generate a new token or access your token (Figure 23).

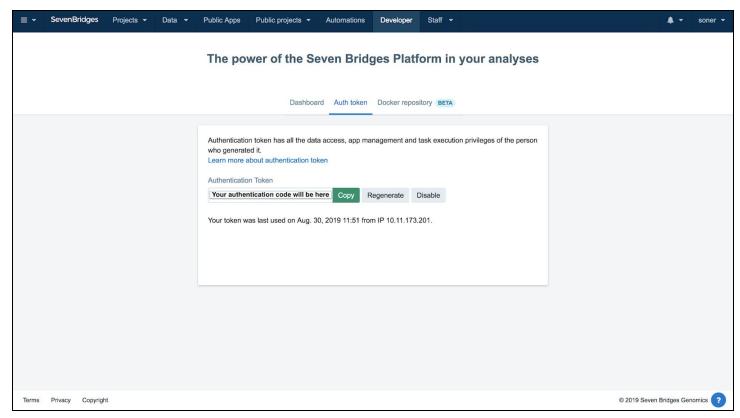


Figure 25: Authentication Token Generation Page of Seven Bridges Platform

Appendix II: BioCompute Object Domains

		BCO Top Level Fields
ID Description		Description
Top Level Fields		
BCO version	bco_spec_version	The version of the BCO specification used to define the BCO.
BioCompute Object Indetifier	BCO_id	Unique identifier that should be apllied to each BCO instance. Assigned by a BCO database engine, like URL. It never be reused.
Checksum	checksum	A string-type, read-only value, protecting the object from internal or external alterations without proper validation.

Table 1: Top Level Fields of BCO

		BCO Provenance Domain
	ID	Description
Provenance Domain		
Name	name	Name of the BCO.
Version	version	Records the versioning of this BCO instance object. A change in the BCO affecting the outcome of the computation should be deposited as a new BCO, not as a new version.
Review	review	Describes the status of an object in the review process. Status flags: unreviewed, in-review, approved, suspended, rejected.
Inheritance/derivation	derived_from	If the object is derived from another, this field will specify the parent object, in the form of the objectid. It is null, if inherits only from the base BioCompute Object or a type definition.
Obsolescence	obsolete	If the object has an expiration date this field will specify that using the datetime type.
Embargo	embargo	If the object has a period of time that it is not public, that range can be specified using these fields. Using the datetime type a start and end time are specified for the embargo.
Created	created	Using the datetime type the time of initial creation of the BCO is recorded.
Modification	modified	Using the datetime type the time of most recent modification of the BCO is recoded.
Contributors	contributors	List to hold contributor identifiers and a description of their type of contribution, including a field for ORCIDs to record author information, as they allow for the author to curate their information after submission.
License	license	A space for Creative commons licence or other licence information. The default or recommended licence can be Attribution 4.0 International.

Table 2: Provenance Domain of BCO

		BCO Usability Domain
	ID	Description
Usability Doma	in	
Usability Domain	usability_domain	Provides a space for the author to define the usability domain of the BCO. It is an array of free text values. This field is to aid in search-ability and provide a specific description of the object. It helps determine when and how the BCO can be used.

Table 3: Usability Domain of BCO

BCO Extension Domain		
	ID	Description
Extension Domain		
Extension Domain	extension_domain	For a user to add more structured information that is defined in the type definition. This section is not evaluated by checks for BCO validity or computational correctness.
Extension to External References: SMART on FHIR Genomics	Extension to External References: SMART on FHIR Genomics	SMART on FHIR Genomics provides a framework for HER-based apps to built on FHIR that integrate clinical and genomics information.
Extension to External References: GitHub	Extension to External References: GitHub	Include an extension to GitHub repositories where HTS computational analysis pipelins, workflows, protocols, and tool or software source code can be stored, deposited, downloaded.

Table 4: Extension Domain of BCO

		BCO Description Domain
	ID	Description
Description Domain		
Description Domain	description_domain	Structured field for description of external references, the pipeline steps, and the relationship of IO objects. Information in this domain is not used for computation. Capture information that is currently being provided in FDA submission in journal format.
Keywords	keywords	List of key map fields to hold a list of keywords to aid in search-ability and description of the object.
External References	xref	It contains a list of the databases and/or ontology IDs that are cross-referenced in the BCO. It provides more specificity in the information related to BCO entries.
Platform/Environment	platform	The multi-value reference to a particular deployment of an existing platform where this BCO can be reproduced (Galaxy or HIVE or CASAVA).
Pipeline tools	pipeline_steps	For recording the specifics of a pipeline. Each individual tool is represented as step, at the discretion of the author. Step Number (step_number), Name (name), Tool Description (description), Tool Version (version), Tool Prerequisites (prerequisite), Input List (input_list).

Tabler 5: Description Domain of BCO

		BCO Execution Domain
	ID	Description
Execution Domain		
Execution Domain	execution_domain	The filelds required for execution of the BCO have been encapsulated together in order to clearly separate information needed for deployment, software configuration, and running applications in a dependent environment.
Script	script	Points to an internal or external reference to a script object that was used to perform computations for this BCO instance. This may be reference to Galaxy Project or Seven Bridges Genomics pipeline, a Common Workflow Language (CWL) object in GitHub, HIVE computational service or any other type of script.
Script Driver	script_driver	The reference to an executable that can be launched in order to perform a sequence of commands described in the script. For example if the pipeline is driven by a HIVE script, the script driver is the hive execution engine. For CWL based scripts specify cwl-runner. Another very general commonly used in Linux based operating systems is shell.
Algorithmic tools and Software Prerequisites	software_prerequisites	Field listing the minimal necessary prerequisites, library, tool versions needed to successfully run the script to produce BCO.
External Data Endpoints	external_data_endpoints	An optional multi-value field listing the minimal necessary domain specific external data source access in order to successfully run the script to produce BCO.
Enviromental Variables	environment_variables	This is an array of key-value pairs useful to configure the execution environment on the target platform.

Table 6: Execution Domain of BCO

	BCO Parametric Domain	
	ID	Description
Parametric Doma	ain	
Parametric Domain	parametric_domain	List of parameters customizing the computational flow which can affect the output of the calculations. These fields are custom to each type of analysis and are tied to a particular pipeline implementation.

Table 7: Parametric Domain of BCO

		BCO Input and Output Domain
	ID	Description
Input and Output Domain		
Input and output Domain	io_domain	This represents the list of global input and output files created by the computational workflow, excluding the intermediate files.
Input Subdomain	input_subdomain	This field records the references and input files for the entire pipeline. Each type of input file is listed under a key for that type.
Output Subdomain	output_subdomain	This field records the outputs for the entire pipeline .

Table 8: I/O Domain of BCO

	BCO Error Domain, acceptable range of variability		
	ID	Description	
Error Domain, ac	ceptable range of	variability	
Error Domain, acceptable range of variability	error_domain	Consists of two subdomains: empirical and algorithmicThe empirical subdomain contains the limits of_detectability_fps, fns, statistical confidence of outcomes, etc. The algorithmic subdomain is descriptive of errors that originated by fuzziness of the algorithms, driven by stochastic processes, in dynamically parallelized multi-threaded executions, or in machine learning methodologies where the state of the machine can affect the outcomeConsists of two subdomains: empirical and algorithmic. The empirical subdomain contains the limits of detectability FPs, FNs, statistical confidence of outcomes, etc. The algorithmic subdomain is descriptive of errors that originated by fuzziness of the algorithms, driven by stochastic processes, in dynamically parallelized multi-threaded executions, or in machine learning methodologies where the state of the machine can affect the outcome.	

Table 9: Error Domain of BCO