WAVES

Web Application for Versatile Enhanced Bioinformatic Services

Marc Chakiachvili [1,2], Sylvain Milanesi [1], Anne-Muriel Arigon Chifolleau [1], Vincent Lefort [1] *

[1] LIRMM, Université de Montpellier, CNRS, Montpellier, France
[2] European Molecular Biology Laboratory, European Bioinformatics Institute, Wellcome Genome Campus, Hinxton, Cambridge, CB101SD, United Kingdom

* Corresponding author: lefort@lirmm.fr

Supplementary Material

DEFINITIONS

Computing infrastructure

Comprized of computationally dedicated hardware and the software components required to operate it, including calculation management programs (distributed resource management systems, Galaxy, other APIs for computation resources...).

Adapter

A component allowing WAVES to communicate with a computing infrastructure.

Service

A bioinformatic tool available online via the http protocol. A service can be accessed from a web form or through REST API calls.

Usage

A list of expected inputs and outputs for a service.

Submission

The combination of a usage and a computing infrastructure. A service can thus rely on different submissions.

Job

Represents a submission run with user-defined values for inputs (files and parameters). A job results in the execution of a command with parameters. It is run on the computing infrastructure defined by the submission. A job generates outputs: exit code, standard output and standard error, and potentially result files.

User

A client accessing services. A client can be a physical person using a web browser, or software using the REST API.

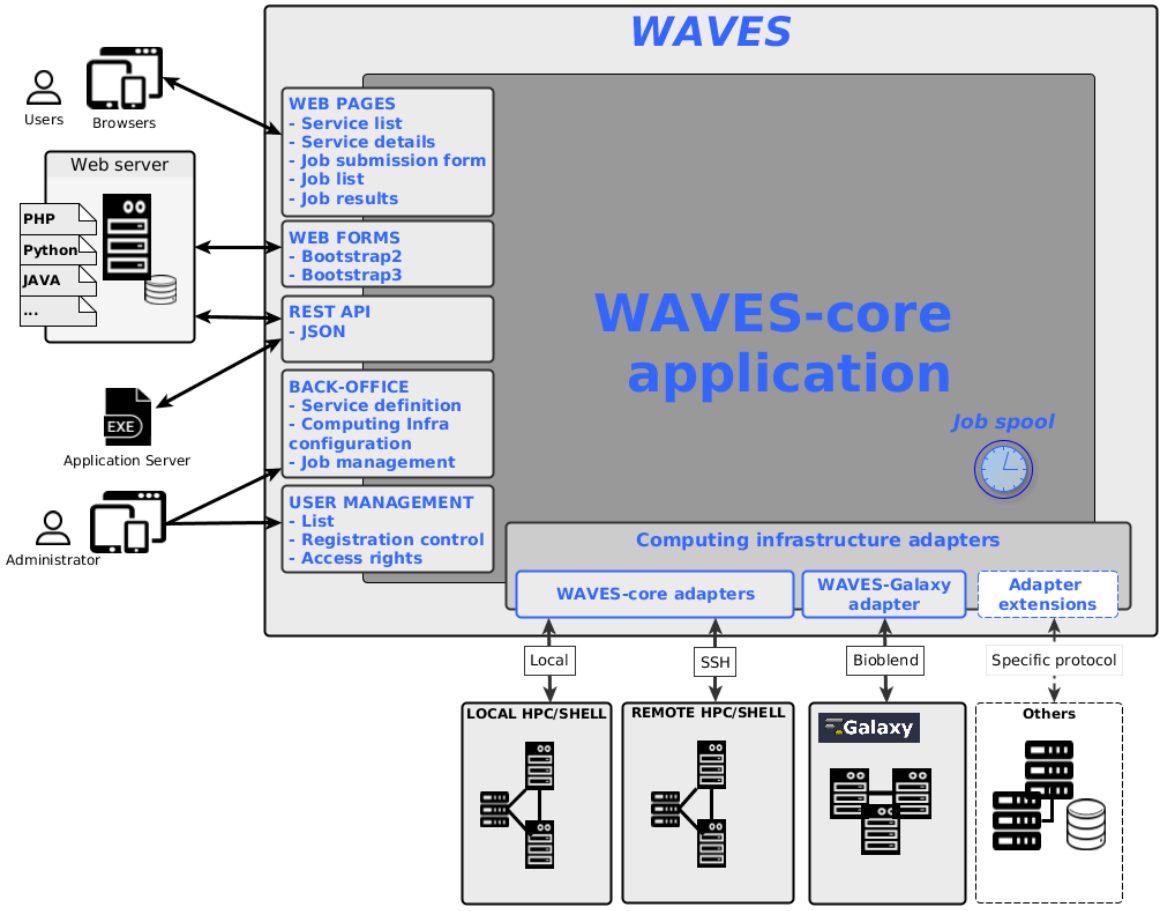
Administrator

A user with access rights to the WAVES back-office. The administrator manages services, submissions, adapters, and jobs.

WAVES architecture

The main goal of WAVES is to facilitate bioinformatic tool integration through web interfaces in order to provide the scientific community with online bioinformatic services. The main WAVES component is called WAVES-core. This component enables administrators to create services that are made available automatically for users. WAVES-core creates web interfaces to provide access to services: web pages and web forms, and REST API entry points (Sup. Fig. 1).

WAVES-core integrates predefined adapters for two types of computing infrastructures: one for command line execution and the other for running jobs on DRMAA-compliant resource management systems. These adapters are designed to be extended to other computing infrastructures. We also provide an extension for Galaxy that is implemented within the WAVES-Galaxy adapter (see dedicated section below).



Sup. Fig. 1. WAVES architecture overview. WAVES is built around WAVES-core, which provides the main WAVES functionalities: user interfaces (“WEB PAGES”, “WEB FORMS” and “REST API”), services and user management (“BACK-OFFICE” and “USER MANAGEMENT”) for administrator use only, and WAVES-core adapters for running jobs on local or remote computing infrastructures. WAVES also includes the WAVES-Galaxy adapter, and can be extended easily to other computing infrastructures by creating dedicated adapters.

WAVES main module: WAVES-core

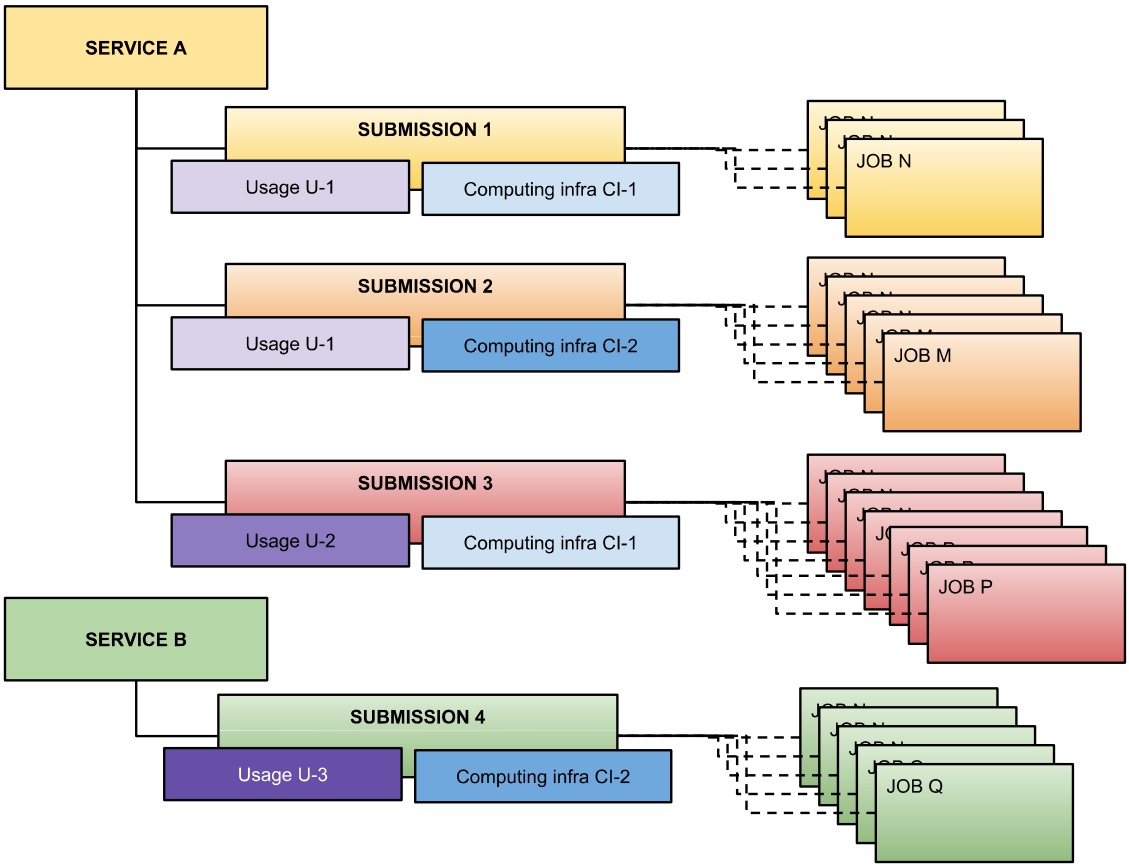
General description

Most of the time, a bioinformatic tool is defined within a single service that relies on a single submission (Sup. Fig. 2, service B). Each user call to a service creates a job that is submitted to the computing infrastructure with specified inputs. WAVES-core then monitors job status during processing on the computing infrastructure. Once the job is terminated, WAVES-core retrieves the results, stores them, and makes them available online via web pages and API entries.

However, some bioinformatic tools provide several distinct usages. For example, a program can be run using a command-line interface or by providing a configuration file. Thus, the same service can provide several usages for the same tool and can be run on several different computing infrastructures. This is done by configuring a submission for each required combination (Sup. Fig. 2, service A).

A standard use case is to define two submissions for the same tool:

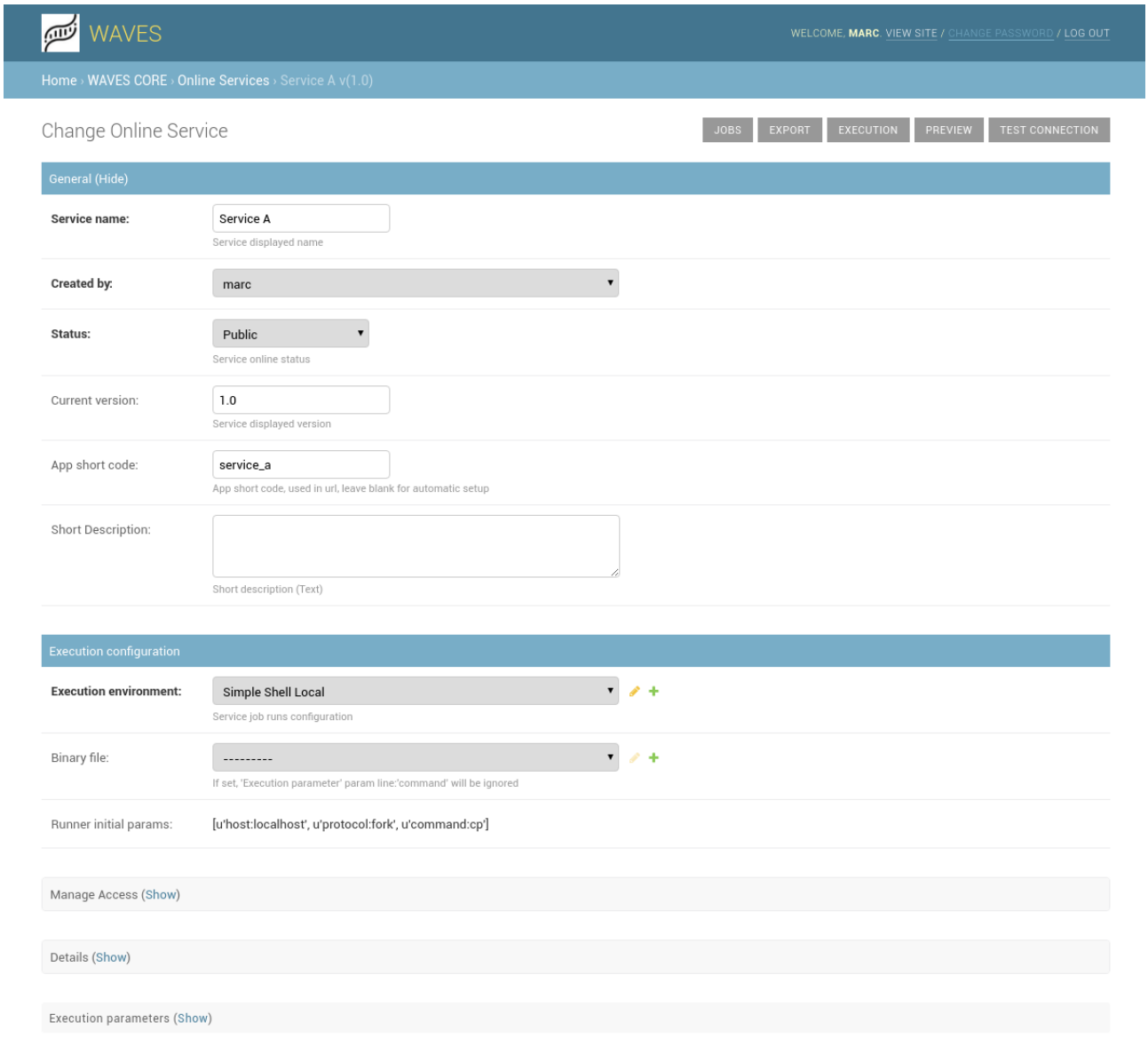
- A default submission with a selection of the most relevant tool parameters with predefined values. This submission is intended to be implemented for inexperienced users.
- An expert submission, which allows fine-tuning of each tool parameter, for advanced users.



Sup. Fig. 2. Service submission model within WAVES.

Service creation

Once installed on a computing infrastructure, a tool is integrated into WAVES by creating and configuring a dedicated service. This is achieved by filling out the ‘Online Service’ form (Sup. Fig. 3) in the WAVES administration interface to define the tool settings. Services can also be imported into WAVES from Galaxy instances and thus automatically configured (see WAVES-Galaxy section below).



Sup. Fig. 3. ‘Online Service’ configuration form from WAVES back-office administration interface.

Service use

There are three different ways to interact with WAVES services: web pages, web forms, and a RESTful API. Example code showing how to interact with a WAVES service web form and API are available from the Developper Guide online documentation.

Service access rules

For each service, the WAVES administrator can setup different access levels (Sup. Table 2).

Service status	Access
Draft	Restricted to service creator
Staff	Access is granted to other WAVES back-office users
Registered	Access is granted to registered users
Restricted	Access is restricted to a selection of registered users
Public	Access is granted to anyone

Sup. Table 1. WAVES services status and corresponding user access rights.

Functionalities

Adapters

By default, WAVES-core comes with predefined adapters to interact with a variety of computing infrastructures (Sup. Table 1). Each adapter parameter is configured by the administrator through the WAVES-core back-office.

Adapter Name	Description
LocalShellAdapter	Execute job with standard shell on Linux-based platform
SshShellAdapter	Connect through SSH protocol with standard credentials user / password on remote server and execute shell command
SshKeyShellAdapter	Connect through SSH protocol using ssh key pairing credentials on remote server and execute shell command
LocalClusterAdapter	Run job on locally installed DRMAA[1] compatible cluster (currently SGE, SLURM, TORQUE, PBS, LSF, CONDOR)
SshClusterAdapter	Connect through SSH protocol with standard user / password credentials on remote DRMAA compatible cluster and run job
SSHKeyClusterAdapter	Connect through SSH protocol using ssh key pairing credentials on remote DRMAA compatible cluster and run job

Sup. Table 2. Predefined WAVES-core adapters for computing infrastructures.

1 http://www.drmaa.org/

Job spool

Once submitted, jobs enter a FIFO (First In First Out) queue to be treated and relayed to the relevant adapter at regular time intervals.

After completion, jobs can be deleted either by administrators or by authorized users. WAVES-core is not intended to be a genuine job queue manager. It relies on an external computation scheduler for performing jobs prioritization and authorization configuration.

Each job may be cancelled by its owner, and WAVES-core then attempts to cancel job execution on the associated computing infrastructure.

User management

Users are managed with the Django standard authentication / authorization mechanism[2], which may be extended to fit any specific requirements for integration. User management allows fine tuning for user access rights.

Users interfaces

Web pages

WAVES-core provides already made front-end web pages, designed with the bootstrap 3[3] CSS framework and using Django standard templating engine[4]. By default, WAVES-core defines the following URIs for accessing its services (Sup. Table 3).

URI	Description
/waves/services/	List all available services
/waves/services/{service_app_name}/	Display service details
/waves/services/{service_app_name}/new	Create a job through submission form(s)
/waves/jobs/{unique_id}/	View job details
/waves/jobs/inputs/{unique_id}/[?export=1]	View input file online / Download file
/waves/jobs/outputs/{unique_id}/[?export=1]	View output file online / Download file

Sup. Table 3. Web page URIs to access WAVES services.

2 https://docs.djangoproject.com/en/1.11/topics/auth/

3 https://getbootstrap.com/

4 https://docs.djangoproject.com/en/1.11/topics/templates/

RESTful API

WAVES-core services are available through RESTful API endpoints. The API lists the available services, and returns service details and associated usages defined within submissions (Sup. Table 4).

METHOD	URI	Description
GET	/waves/api/services	List all available services
GET	/waves/api/services/{service_app_name}	Retrieve service details
GET	/waves/api/services/{service_app_name}/form	Retrieve service forms (for all submissions)
GET	/waves/api/services/{service_app_name}/jobs	Retrieve service jobs (only for logged-in users)
GET	/waves/api/services/{service_app_name}/submissions	List all available submissions for this service
GET	/waves/api/services/{service_app_name}/submissions/{submission_app_name}	Get detailed service submission information (inputs, parameters, expected outputs)
GET	/waves/api/services/{service_app_name}/submissions/{submission_app_name}/jobs	List all user jobs for this submission
POST	/waves/api/services/{service_app_name}/submissions/{submission_app_name}/jobs	Create a new job from submitted inputs
GET	/waves/api/services/{service_app_name}/submissions/{submission_app_name}/form	Get HTML submission form that submits data to the above “POST” URI

Sup. Table 4. WAVES-core services REST API endpoints. The "POST" method is only accessible through authenticated requests, while "GET" method can be accessed anonymously.

WAVES-core provides REST API endpoints to follow the job execution life cycle and retrieve results once terminated (Sup. Table 5).

METHOD	URI	Description
GET	/waves/api/jobs	List all available user job summaries, with related detailed URI
GET	/waves/api/jobs/{unique_id}	Detailed job information, allows direct link to submitted inputs, results outputs, status history, related submission and service
GET	/waves/api/jobs/{unique_id}/status	Retrieve job status
GET	/waves/api/jobs/{unique_id}/inputs	List job inputs
GET	/waves/api/jobs/{unique_id}/inputs/{api_name}	Retrieve input content (for file)
GET	/waves/api/jobs/{unique_id}/outputs	List job outputs
GET	/waves/api/jobs/{unique_id}/outputs/{api_name}	Retrieve output file content
POST	/waves/api/jobs/{unique_id}/cancel	Cancel job and tag it as cancelled
DELETE	/waves/api/jobs/{unique_id}	Delete job

Sup. Table 5. WAVES-core REST API endpoints for job management. All methods require an authenticated request.

The WAVES-core API is compatible with Core API[5] specifications. Thanks to Django REST framework[6], WAVES implements the Core JSON schema which can be browsed from WAVES-demo[7].

Other WAVES module: WAVES-Galaxy

Using the BioBlend[8] python library, this adapter enables Galaxy services import into WAVES-core. WAVES-Galaxy[9] automatically recognizes the tools available in a Galaxy instance. The WAVES administrator can select the tools to integrate within the back-office. WAVES-Galaxy then creates a new service for each selected Galaxy tool automatically. When called from WAVES, each submission of this service is run on the Galaxy instance from which it was imported.

5 http://www.coreapi.org/

6 http://www.django-rest-framework.org/api-guide/schemas/

7 http://waves.demo.atgc-montpellier.fr/waves/api/schema

8 http://bioblend.readthedocs.io/

9 http://waves-galaxy-adaptors.readthedocs.io/

Licensing

Django and its components are open-source software, developed by a large community (more than 10,000 people) and benefiting from a wide range of reusable packages.

WAVES has been made available on GNU Public License version 3[10], meaning that anyone may use, reuse, and modify the code. We invited people to help us make WAVES even better, so don't hesitate to participate in the project on GitHub.

Useful links

WAVES-core

- GitHub repository: https://github.com/lirmm/waves-core
- Documentation: http://waves-core.readthedocs.io

WAVES-demo

- GitHub repository: https://github.com/lirmm/waves-demo
- Documentation: http://waves-demo.readthedocs.io
- Example: http://waves.demo.atgc-montpellier.fr/

WAVES-galaxy adapter

- GitHub repository: https://github.com/lirmm/waves-galaxy
- Documentation: http://waves-galaxy-adaptors.readthedocs.io

SAGA python framework

- GitHub repository: https://github.com/radical-cybertools/saga-python
- Documentation: http://saga-python.readthedocs.io
- Project home: https://radical-cybertools.github.io

10 https://www.gnu.org/licenses/gpl.html