

SHaring Interoperable Workflows for Large-Scale Scientific Simulations on Available DCIs

Workflow Interoperability Enables Interdisciplinary Research

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02nd February 2012**



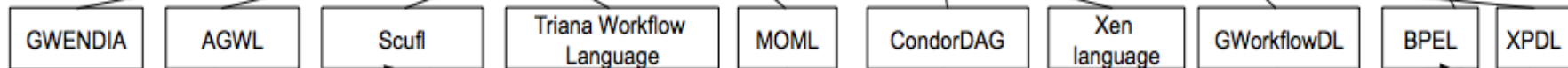


Workflow Interoperability Challenge

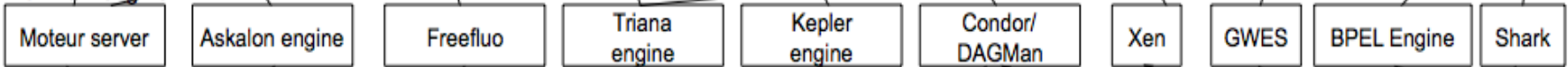
Workflow Formalism



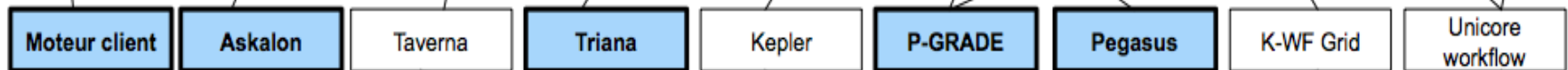
Workflow Language



Workflow engine



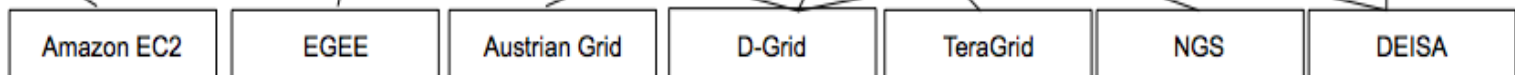
Workflow system



DCI middleware



DCI infrastructures





SHIWA Project

Partners:

Computer and Automation Research Institute, Hungarian Academy of Sciences

[MTA SZTAKI](#)

Hungary

University of Innsbruck

[UIBK](#)

Austria

Charité - Universitätsmedizin Berlin

[C-UB](#)

Germany

French National Centre for Scientific Research

[CNRS](#)

France

University of Westminster

[UOW](#)

United Kingdom

Cardiff University

[CU](#)

United Kingdom

Academic Medical Centre of the University of Amsterdam

[AMC](#)

Netherlands

University of Southern California

[USC](#)

USA



Duration:

July 2010 – June 2012 (extended to September 2012)



SHIWA Objectives and Services

Objectives:

- To create an environment which enables seamless execution of workflows of different workflow systems through workflow interoperability

Services:

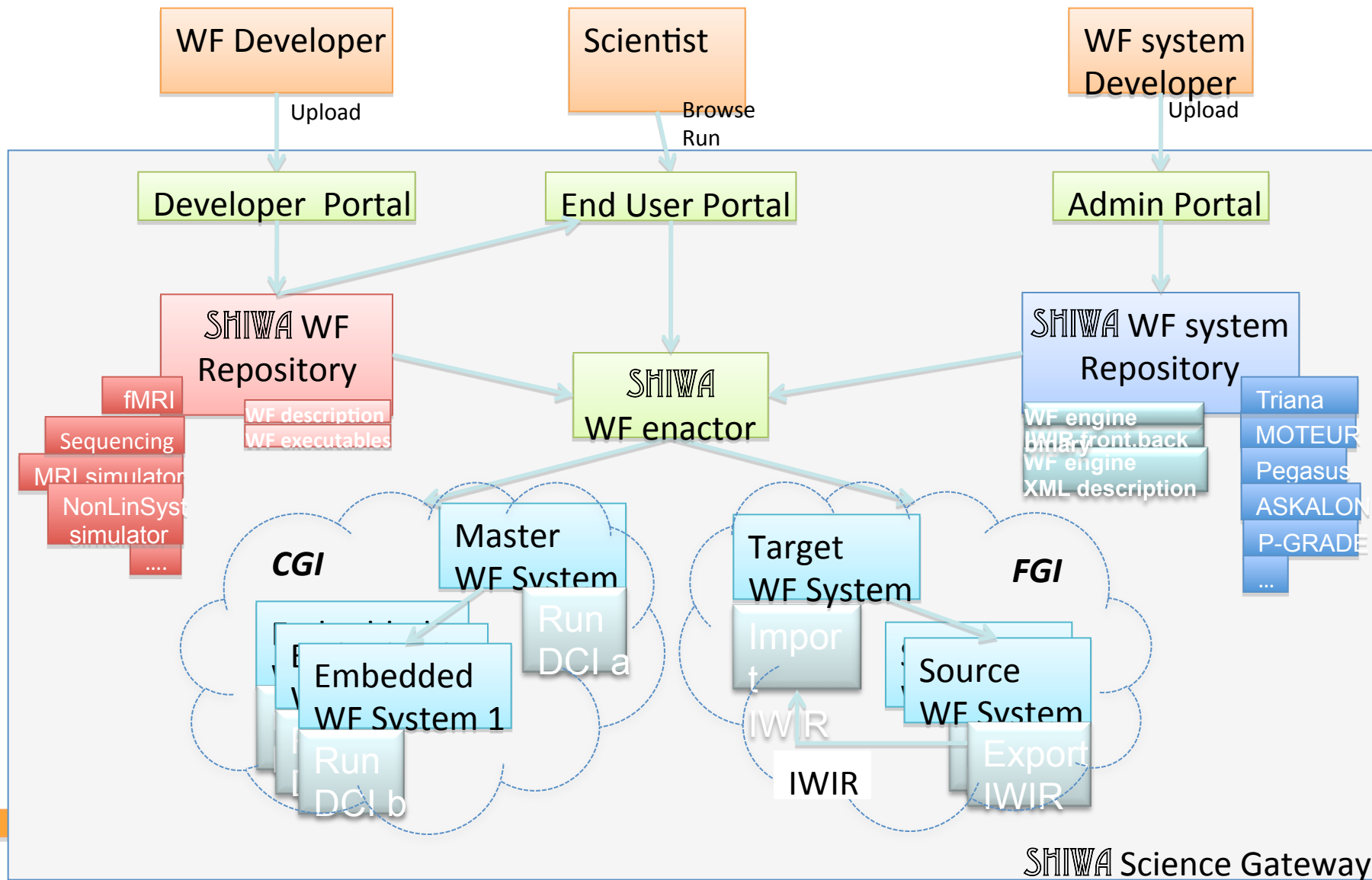
- supports the whole workflow lifecycle: editing, uploading, browsing downloading and executing workflows
- provides coarse- and fine-grained workflow interoperability solution
- offers Distributed Computing Infrastructure interoperability solution
- provides desktop computer and portal interfaces to manage workflows

Key actors:

- researchers
- workflow engine developers
- workflow developers

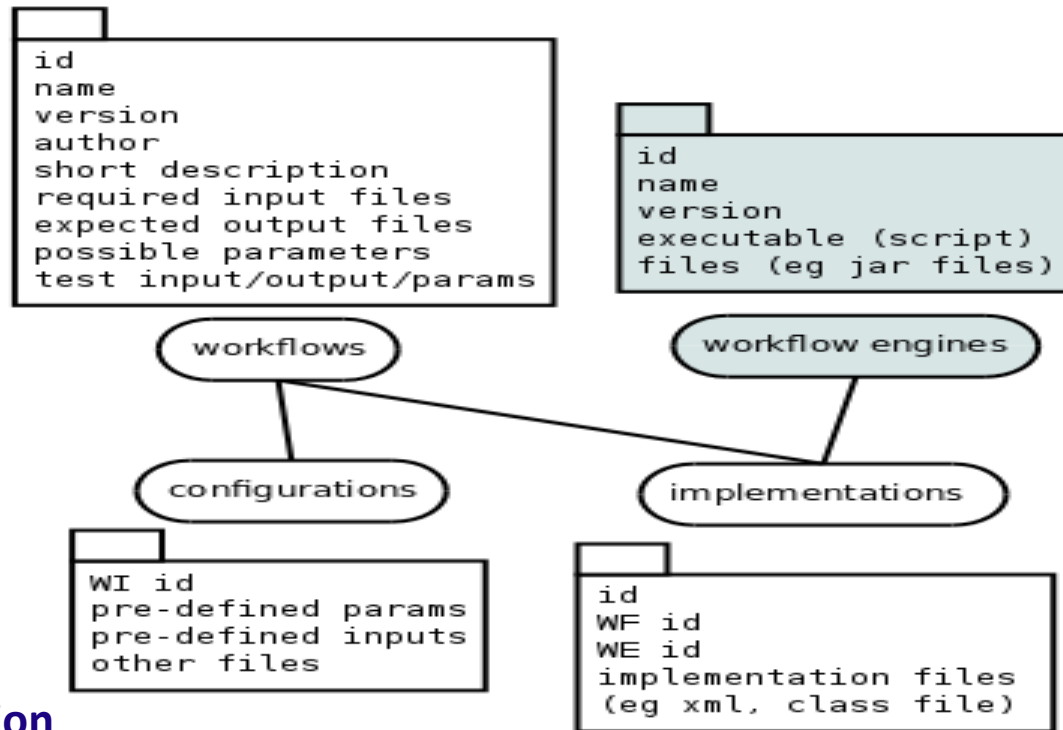


SHIWA Solution





SHIWA Data Structure



Workflow description

- plain text which describes the inputs and outputs and explains what the workflow does

Workflow implementations

- It contains all implementation files or references to these files (via eg. URLs) and also holds other data/metadata necessary to run the workflow on its associated workflow engine.

Workflow configurations

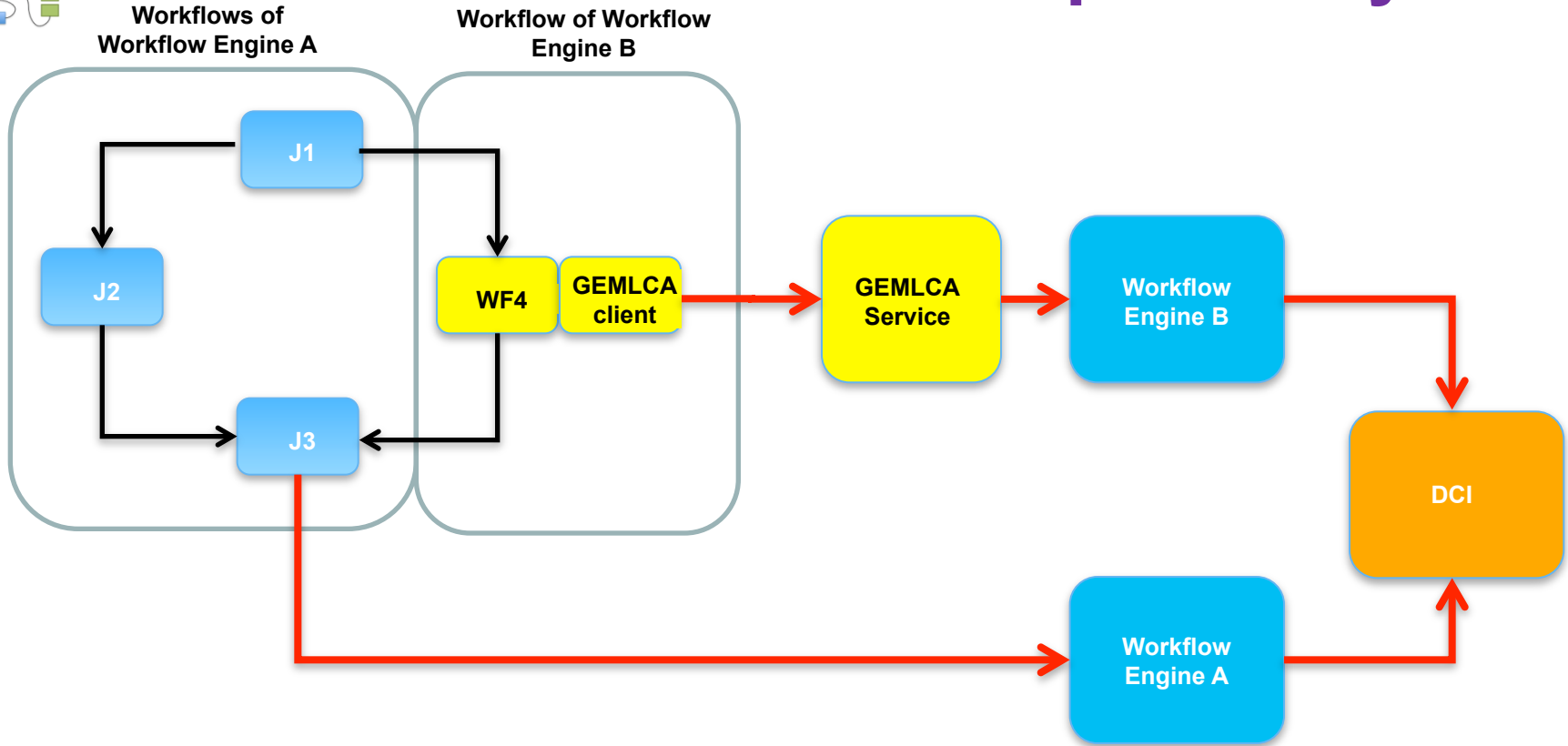
- It contains pre-defined input files and parameters or references to these files and parameters and other data/metadata of a workflow.

Workflow engines

- It contains files and other data/metadata necessary to execute a workflow engine on a grid site or references to them



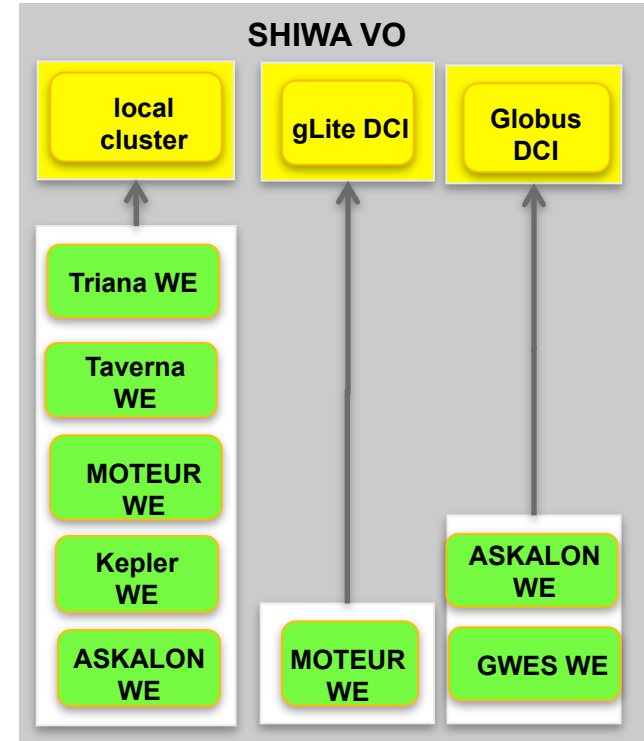
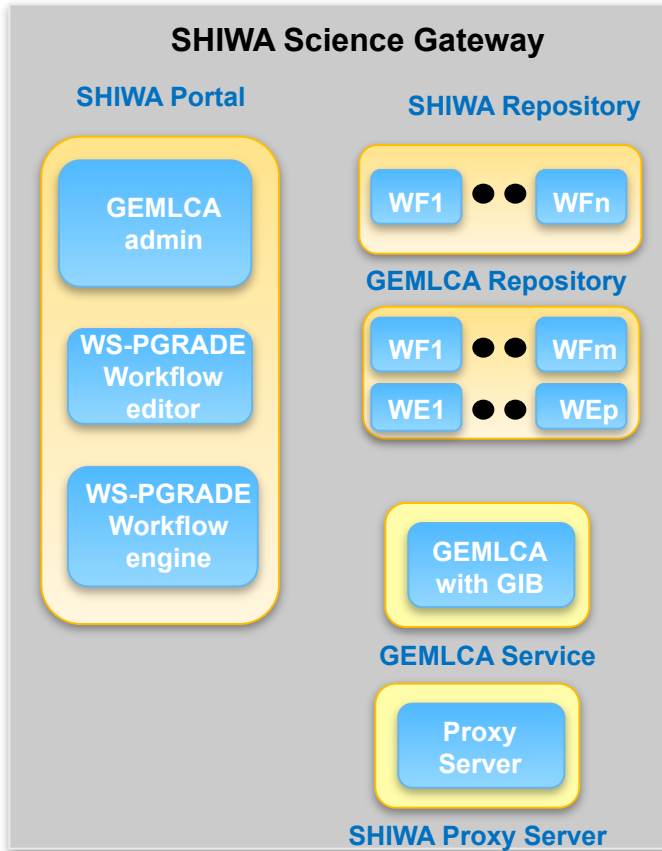
Coarse-Grained Interoperability



- **native workflows:** J1, J2, J3
- **non-native workflows:** WF4
- **black boxes which are managed as legacy code applications**



CGI Infrastructure



SHIWA Science Gateway

native WE portal	PGRAD
repository	PGRAD v2.4.1
submitter	GEMLCA + SHIWA repo
proxy management	GEMLCA with GIB
	SHIWA Proxy Server

Resources

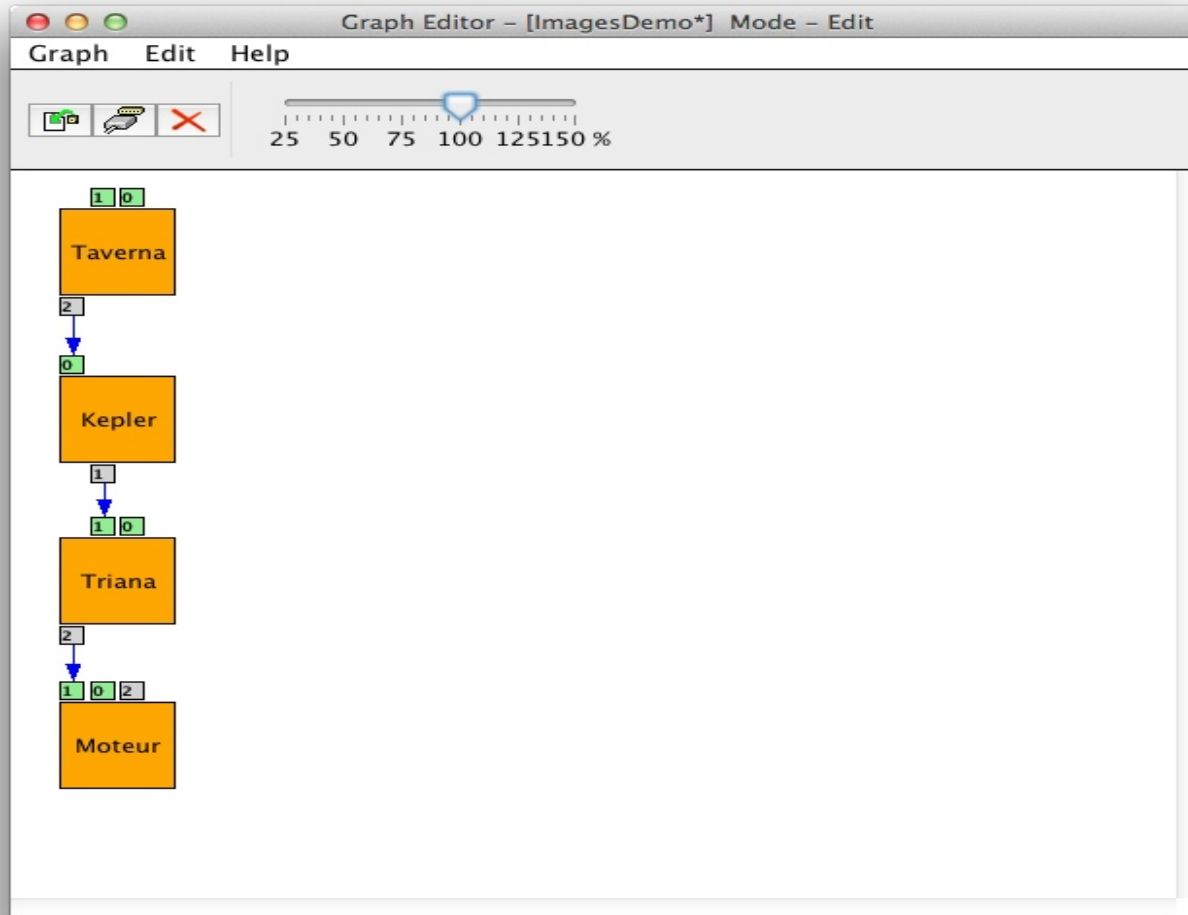
local resources: invocation of locally deployed WEs
 WE submission to local cluster

remote resources: through remotely pre-deployed WEs to gLite and Globus DCIs

pre-deployed-WEs



SHIWA Portal: Workflow Editor





SHIWA Portal: Configuring Workflow

shiwa-portal.cpc.wmln.ac.uk > Workflow > Concrete

Moteur

Selected job to be configured

Job's name: Kepler
Optional note: Description of Job



[Job Executable]



[Job I/O]



[DDL/RSL]



[History]

Job execution model:



Interpretation of the job as a Workflow



Interpretation of the job as a Binary

Type

GEMMLCA Repository:

Service Method:

Resource:

GEMMLCA parameters: 1 input 1 output port(s)

Do not forget to configure the file associations in the Job Inputs and Outputs tab

Save.. Quit

- CIVETPipeline-neugrid: CIVET-LINGA-LonWS-neugrid
- FreeSurfer-LONI-cranium: FreeSurfer-cranium
- GateAdaptors: Gate Adaptors with command line for WE
- Kepler-WF1g: Workflow 1 via GIB
- Kepler-WF2g: Workflow 2 via GIB
- dummy-civet: dummy-civet
- merlin2g: Merlin multiparam Kepler via GIB
- testAd: Gate Adaptors with command line for WE
- testbashgib: Simple catter script



SHIWA Portal: Executing Workflow

[shiwa-portal.cpc.wmin.ac.uk](#) > [Workflow](#) > [Concrete](#)

Concrete



[Back](#)
[Refresh](#)

Workflow name: Images-Demo-c1
 Note: 2011-8-22
 Workflow Graph: ImagesDemo
 Workflow Template: --

2011-8-23 9:36	finished	Details	Delete
2011-11-24 8:1	running	Details	Suspend
2011-9-9 9:51	finished	Details	Delete
2011-9-9 9:12	finished	Details	Delete
2011-8-22 10:24	finished	Details	Delete
2011-9-12 10:34	finished	Details	Delete

Selected WF Instance:

2011-11-24 8:1

Job	Status	Instances	[Actions]
Moteur	init	1	View init View all content(s)
Taverna	running	1	View running View all content(s)
Kepler	init	1	View init View all content(s)
Triana	init	1	View init View all content(s)



SHIWA Workflow Repository

Home Workflows Implementations Users Groups Engines User Manual Log out

Filters

Workflows **Browse Workflows** **Browse Implementations** **Advanced Search**

25 (1 of 2)

Name	Owner	Group	Description
SolidBwaAlignment	vladimir	BWA	Burrows-Wheeler Aligner (BWA) workflow: - Conve...
MeanShift		Creations	The Meanshift application is
simriMPI	fredj	CreatisSimri	SIMRI is an MR simulator based on the Bloch e...
simriMetaWorkflow	fredj	CreatisSimri	This meta-workflow shows how to use different i...
test	ibrahim	css	workflow test
DTIAtlasCoreg	vladimir	DTIAtlas	DTI Atlas Coregistration: Spatial corresponen...
DTIAtlasWarp	vladimir	DTIAtlas	DTI Atlas Warp: The deformation fields computed...
DTIAtlasFit	vladimir	DTIAtlas	DTI Atlas Fit: estimates orientations in each v...
DTIAtlasMetaWf	vladimir	DTIAtlas	DTI Atlas meta workflow: Magnetic Resonance Ima...
BronzeStandard	tram	Examples	This is the Bronze Standard workflow. It consis...
FSLBedpostX	vladimir	FSLBedpostX	FSL BedpostX: The FMRIB Software Library (FSL) ...
FSLBedpostXMetaWF	vladimir	FSLBedpostX	FSL BedpostX meta workflow: consists of FSL Bed...
PreparationGateWF	fredj	GateWF	This workflow splits a GATE simulation in 3 par...
mergeWF	fredj	GateWF	The merge process of GATE simulation.
metaGATE	fredj	GateWF	The meta workflow of GATE simulation has 8 nes...
GateSimulation	fredj	GateWF	GATE is a simulation software developed by the ...



SHIWA Workflow Repository

★ Welcome 🏠 Home 📁 Workflows ▾ ⚙️ Implementations ▾ ✎ Administration ▾ ? Documentation ▾ ✕ Log out

Find Workflows

All Domains ▾

subtraction

Search

Show All

Refresh

(1 of 1)



1



10 ▾

Workflow: SimpleWF_IntegerSubtractor

Edit

Details

Workflow Summary

Domain: Demonstration

Application: demonstration

Owner: [Tamas Kukla](#)

Group: shiwaExampleWfs

Keywords: subtraction, integer

Description: This workflow subtracts two integers and outputs the result. The input integers are provided in text files and the result is also a text file containing the difference. This workflow serves demonstration purposes.

Inputs (2) +

Outputs (1) +

Data sets (2) +

Implementation Preview (2)

Kepler Subtract 1.0



Engine: Kepler(1.0)

Version: 1.0

DCIs: SHIWA VO

Keywords: Kepler, local, subtract, integer

Description: This workflow is executed locally to the Kepler engine.

[Edit](#)

Kepler Subtract 1.1



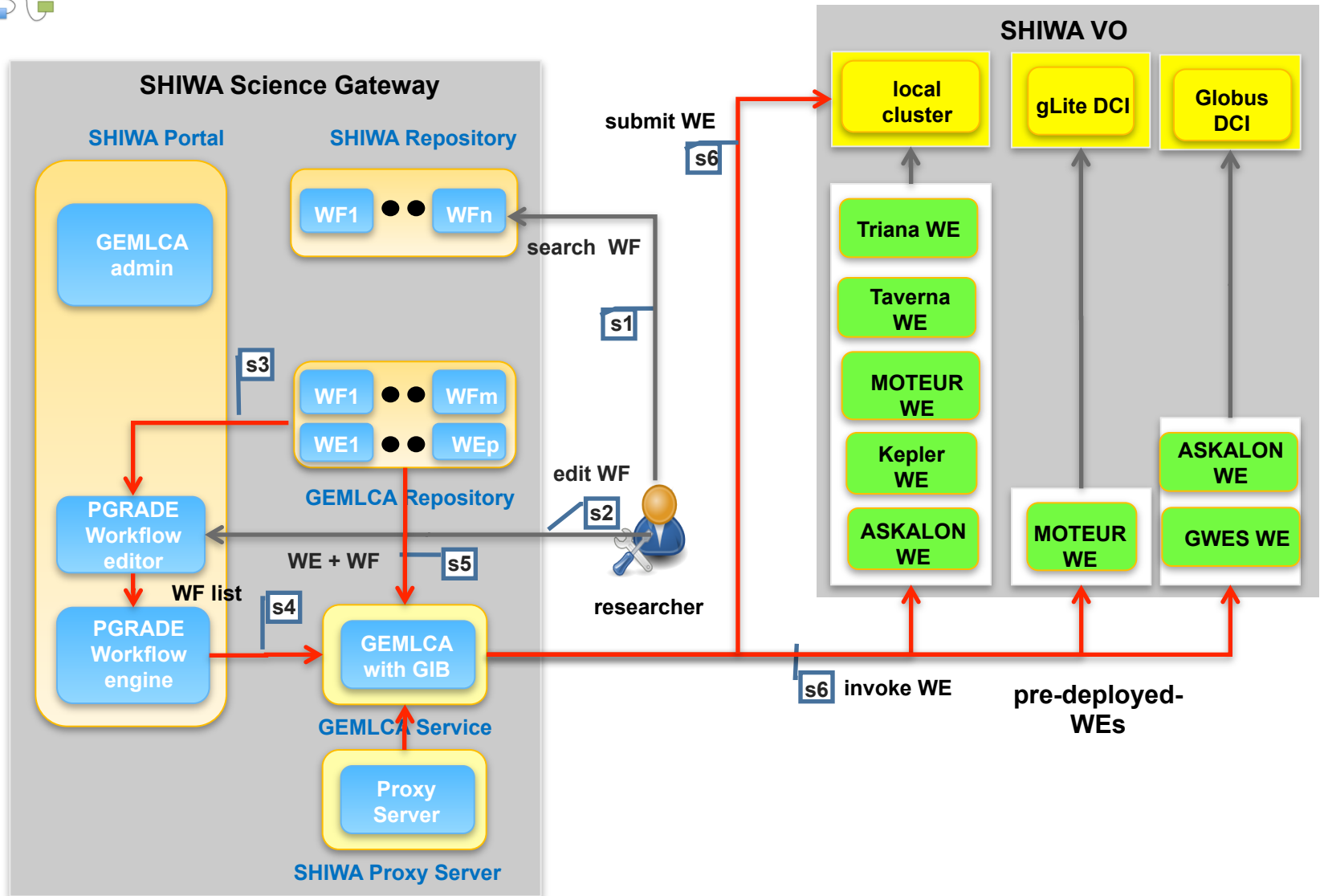
Engine: Kepler(1.0)

Version: 1.1

DCIs: SHIWA VO

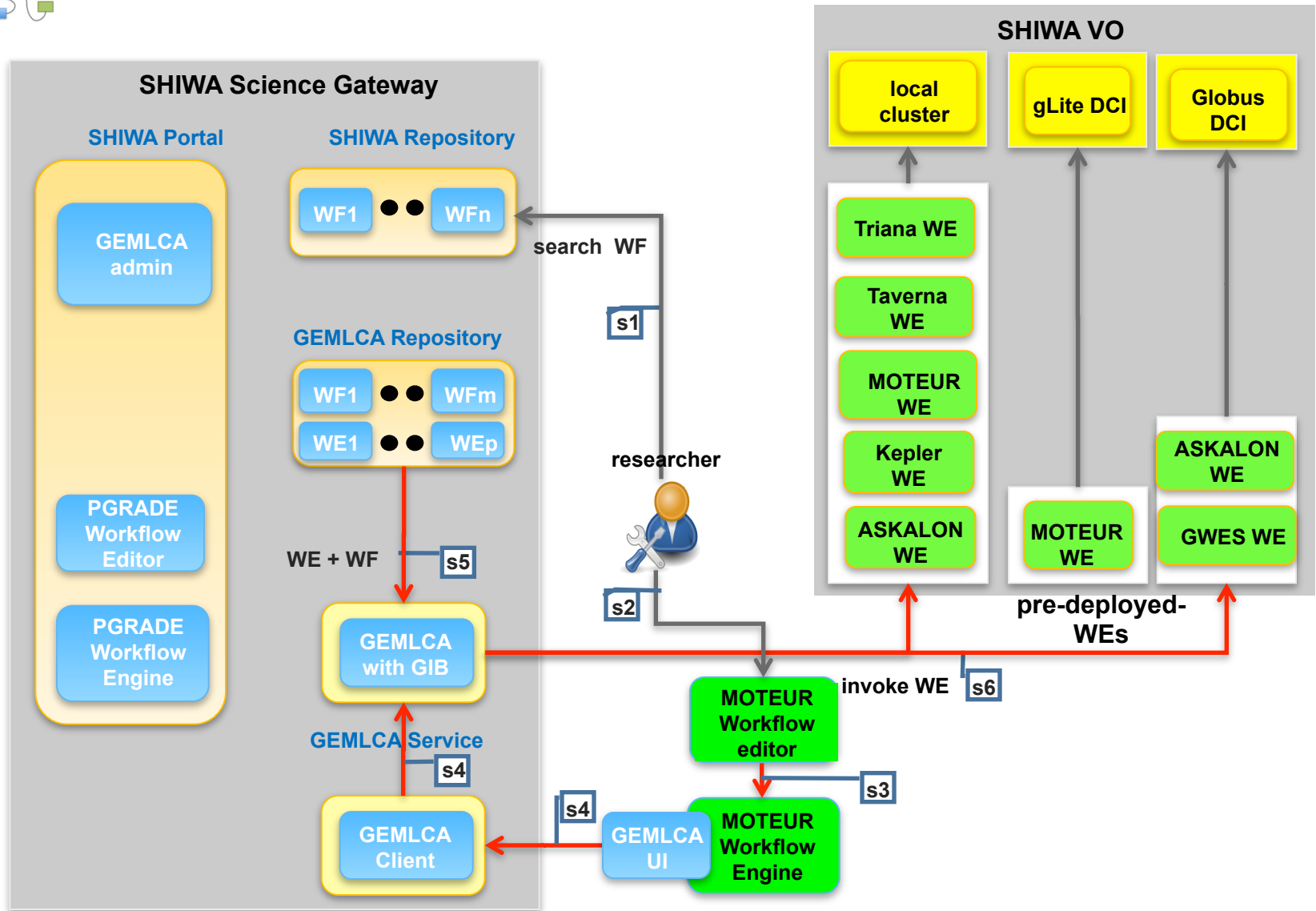


CGI User Scenario: Native WE



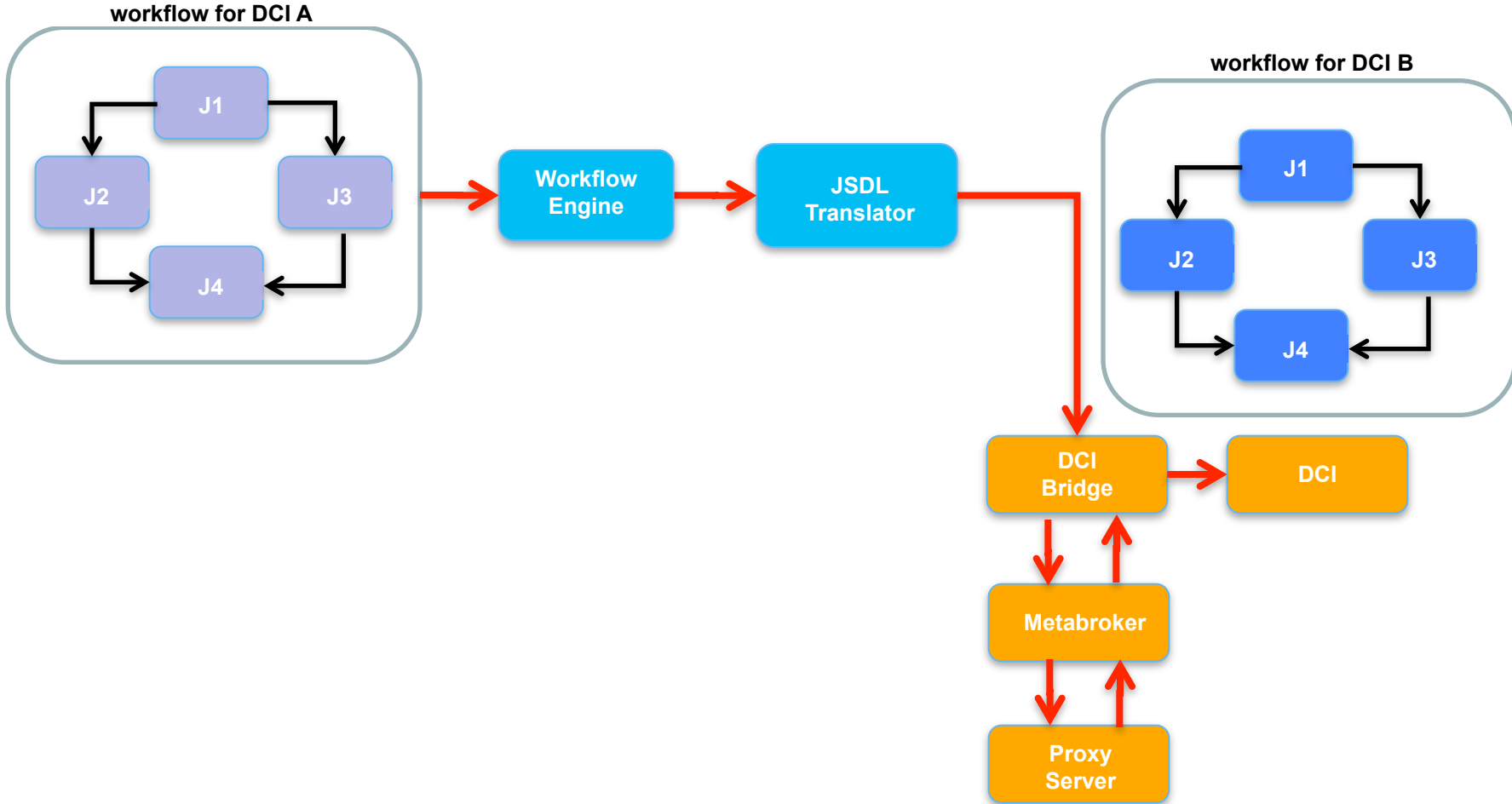


CGI User Scenario: Non-native WE

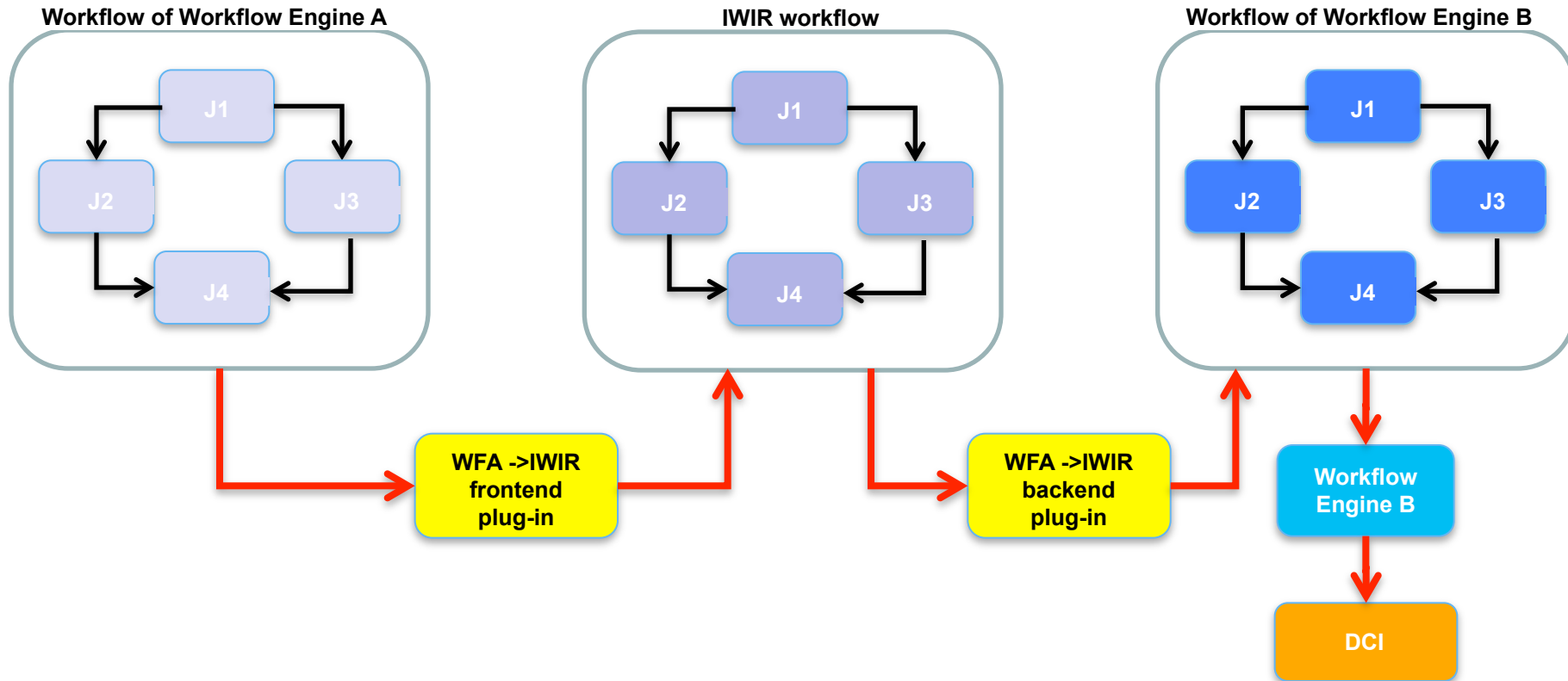




DCI Interoperability



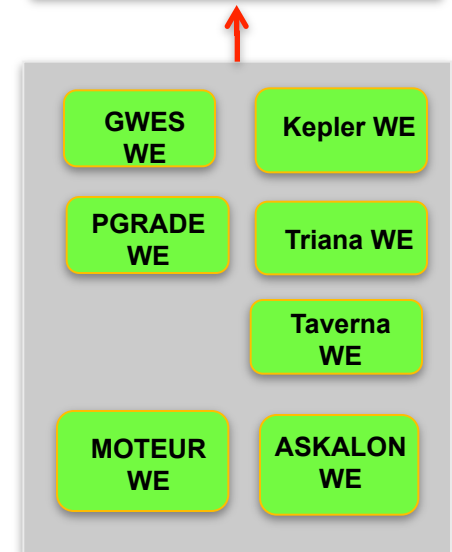
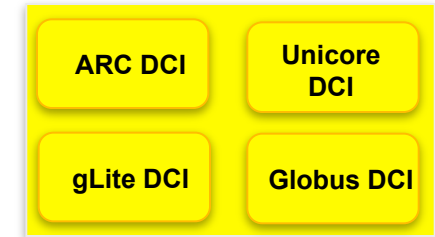
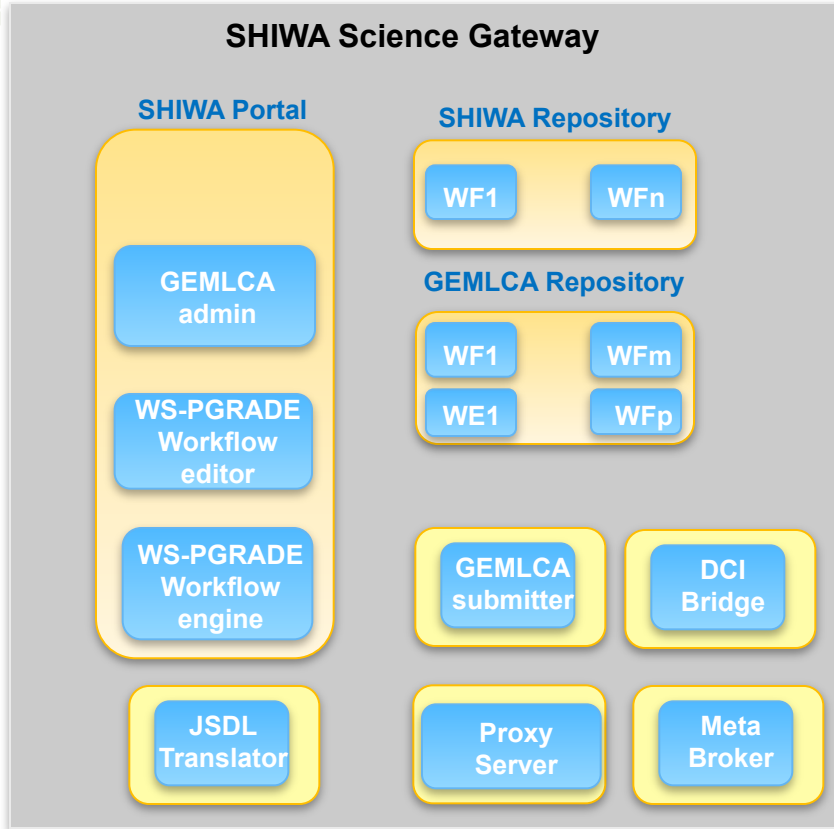
Fine-Grained Interoperability



- front-end plug-in: converts workflow of workflow engine A into IWIR representation
- back-end plug-in: converts from IWIR representation into workflow of workflow engine B



SSP DCI & FGI Infrastructure DCIs



SHIWA Science Gateway

Resources

native WE
portal
repository
GEMLCA
proxy server

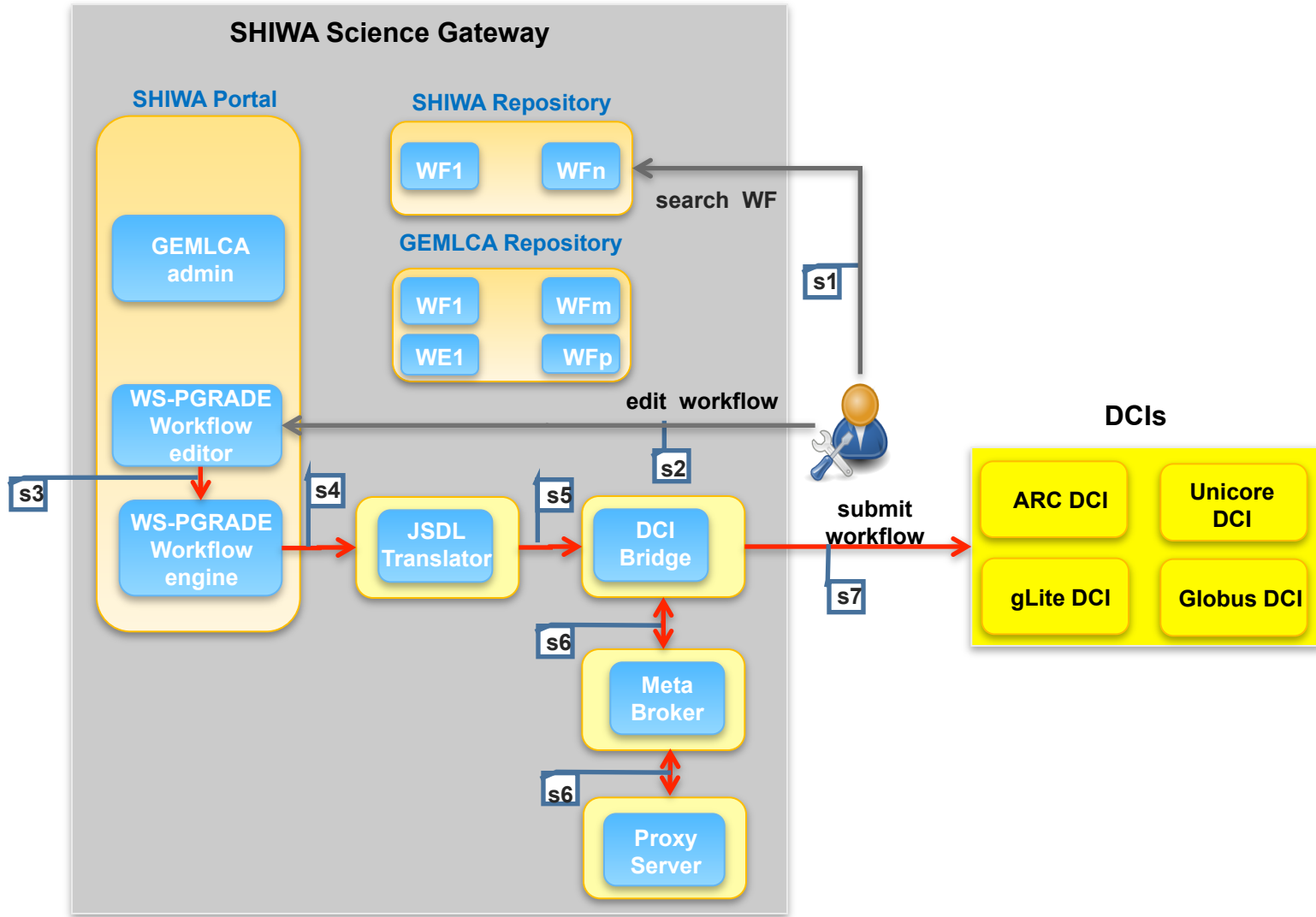
ASKALON, MOTEUR, WS-PGRADE
WS-PGRADE v3.2.2
GEMLCA + SHIWA

local WEs: Kepler, MOTEUR, Taverna & Triana WEs
submit to the local cluster

remote WEs: ASKALON, GWES & MOTEUR WEs
ARC, gLite, Globus and Unicore DCIs

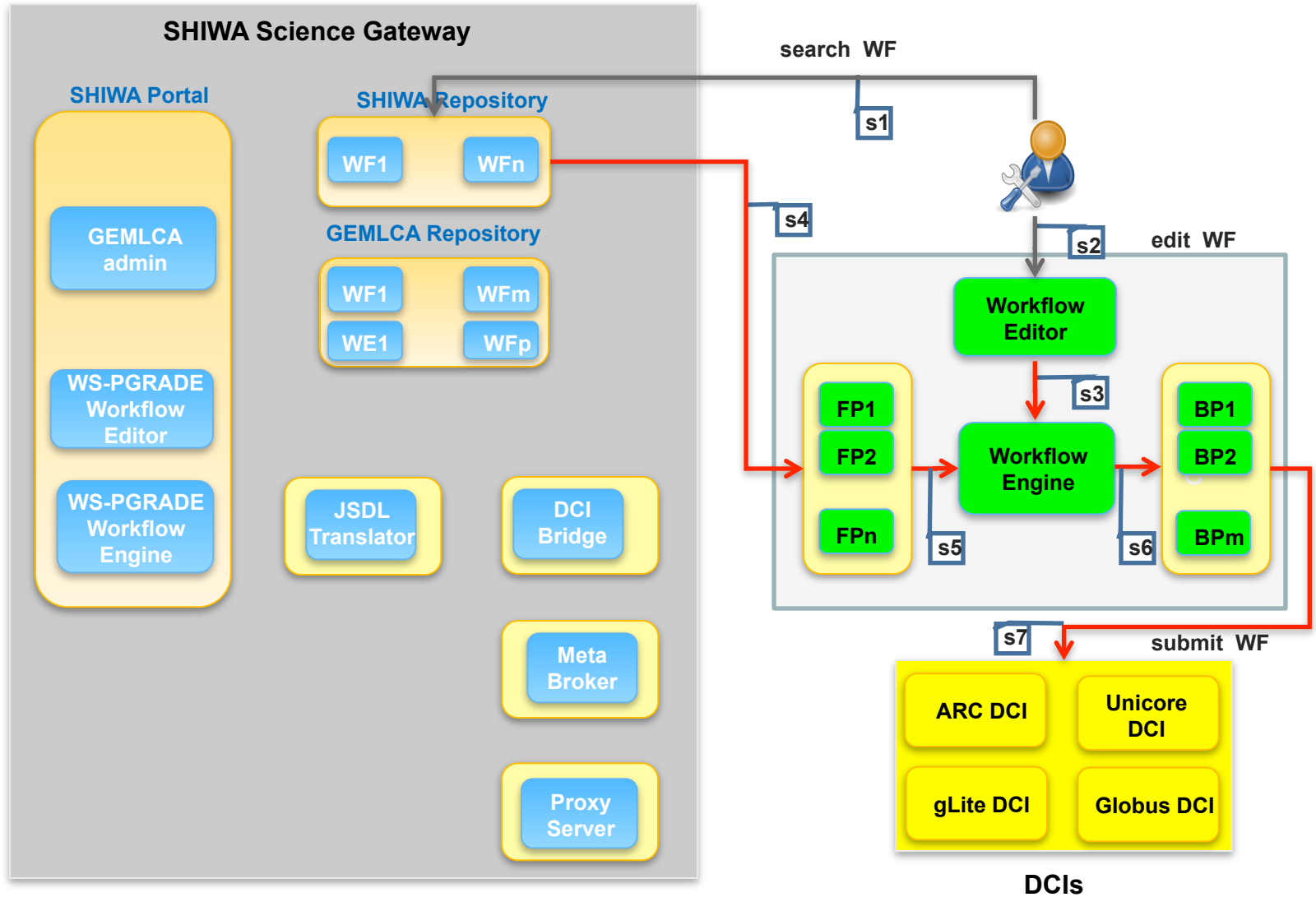


DCI Interoperability Scenario





FGI Interoperability Scenario





SHIWA Simulation Platform: Access

SHIWA Science Gateway (SHIWA Portal + SHIWA Repository)

- portal and repository account given by the science gateway administrator

DCI resources

- certificate given by the relevant DCI administrator, for example the VO sysadmin

Access to the SHIWA Portal

shiwa-portal.cpc.wmin.ac.uk/liferay-portal-6.05

Access to the SHIWA Repository

shiwa-repo.cpc.wmin.ac.uk



SHIWA Simulation Platform: Selling Points

- the simulation platform supports the **whole lifecycle of workflows**, i.e. creating, testing, uploading, browsing, downloading and running workflows
- users can use workflows of their own and of other workflow systems through the same user interface, i.e. they can re-cycle or **share workflows** created by other research teams or even other research communities
- **workflow developers** (or e-scientists) can create, run, upload workflows through the simulation platform
- **researchers** (astro physicists, earth scientists, bio scientists, etc.) can browse the workflow repository, select and run workflows through the simulation platform
- the simulation platform provides access to major **European e-infrastructure**, the European Grid Initiative (EGI) infrastructure which offers large pool of compute and storage resources