BioVeL

A "Software as a Service" solution for exploiting Grid/ Cloud infrastructure for bioinformatics and biomedical analysis workflows

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INFN-Bari

Biodiversity Virtual e-Laboratory

BioVeL is an international network of experts

- Connects two scientific communities: IT and biodiversity.
- Offers an international network of IT expert scientists in BioVeL's data processing services.
- Shares expertise in workflow studies among BioVeL's users.
- Fosters an international community of researchers and partners on biodiversity issues.
- BioVeL is an e-laboratory that supports research on biodiversity using large amounts of data from cross-disciplinary sources.

Biodiversity Virtual e-Laboratory

BioVeL is a consortium of 15 partners from 9 countries

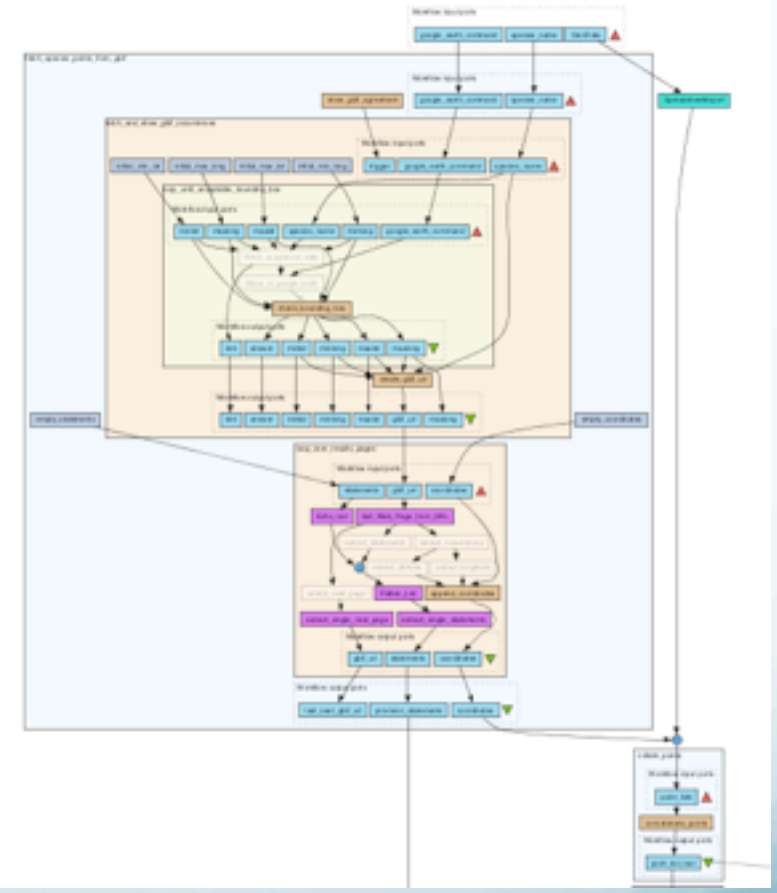
1. Cardiff University, UK – Coordinator
2. Centro de Referência em Informação Ambiental, Brazil
3. Foundation for Research on Biodiversity, France
4. Fraunhofer-Gesellschaft, Institute IAIS, Germany
5. Free University of Berlin – Botanical Gardens and Botanical Museum, Germany
6. Hungarian Academy of Sciences Institute of Ecology and Botany, Hungary
7. Max Planck Society, MPI for Marine Microbiology, Germany
8. National Institute of Nuclear Physics, Italy
9. National Research Council: Institute for Biomedical Technologies and Institute of Biomembrane and Bioenergetics, Italy
10. Netherlands Centre for Biodiversity (NCB Naturalis), The Netherlands
11. Stichting European Grid Initiative, The Netherlands
12. University of Amsterdam, Institute of Biodiversity and Ecosystem Dynamics, The Netherlands

13. University of Eastern Finland, Finland
14. University of Gothenburg, Sweden
15. University of Manchester, UK

Biodiversity Virtual e-Laboratory

BioVeL is a powerful data processing tool

- Import data from one's own research and/or from existing libraries.
- "Workflows" (series of data analysis steps) allow to process vast amounts of data.
- Build your own workflow: select and apply successive "services" (data processing techniques.)
- Access a library of workflows and re-use existing workflows.
- Cut down research time and overhead expenses.
- Contribute to LifeWatch and GEO BON.



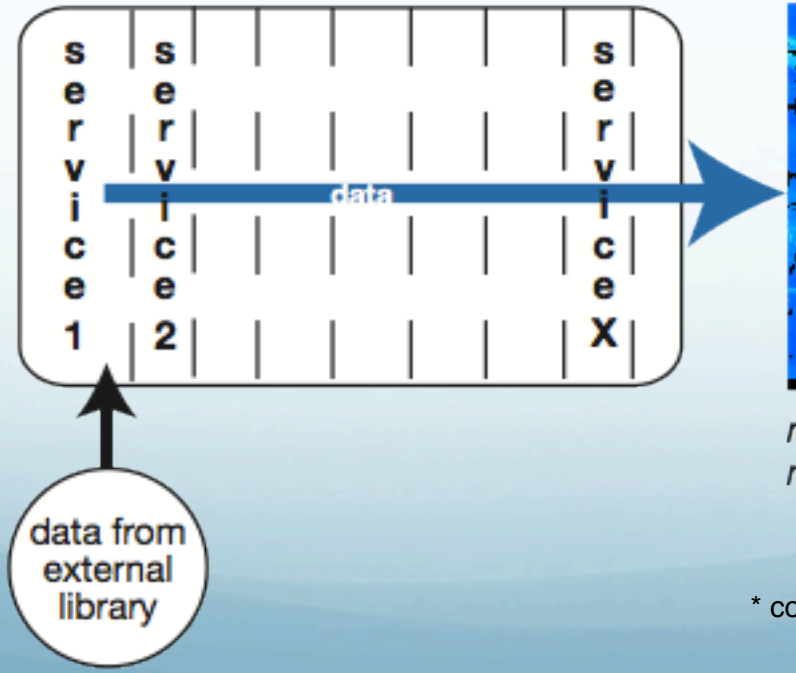
Part of a workflow to study the ecological niche of the horseshoe crab

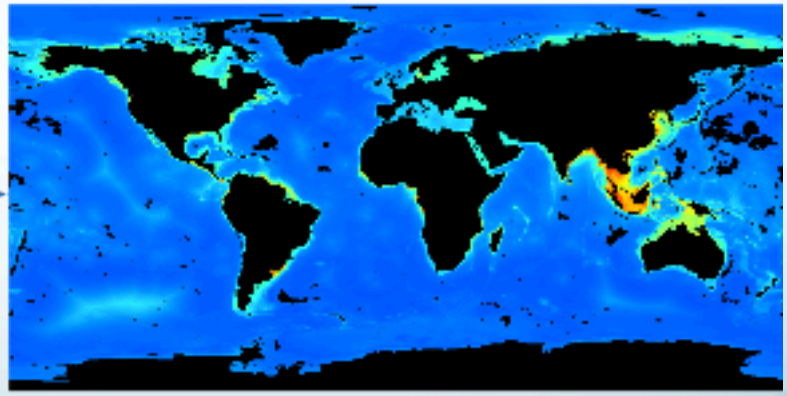
Biodiversity Virtual e-Laboratory

Showcase study 1: <u>create</u> a workflow*

Study on the ecological niche of the south east Asian horseshoe crab, an endangered species:

- Import south east Asian data from external library
- Apply succession of "services" = workflow
- Result: ecological niche map





results: map showing the potential ecological niche of the south-east Asian horseshoe crab

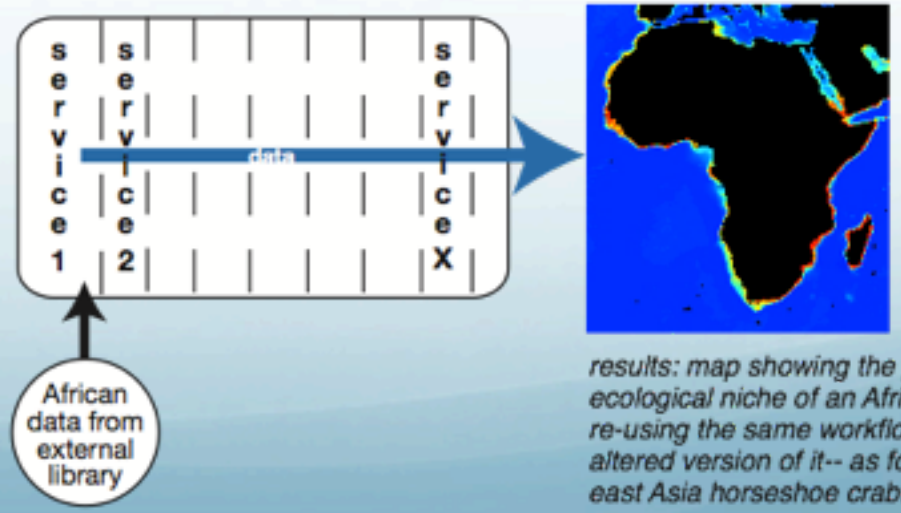
* courtesy Matthias Obst, University of Gothenburg, Sweden

Showcase study 2: re-use a workflow

Study on the ecological niche of the American horseshoe crab
- Import American data
- Re-use south east Asia crab study workflow
- Result: ecological niche map for American horseshoe crab

Compare the ecological niches of the south east Asian and American crabs.

Potential study of the ecological niche of an African animal
- Import African data
- Re-use horseshoe crab study workflow
- Result: ecological niche map for African animal

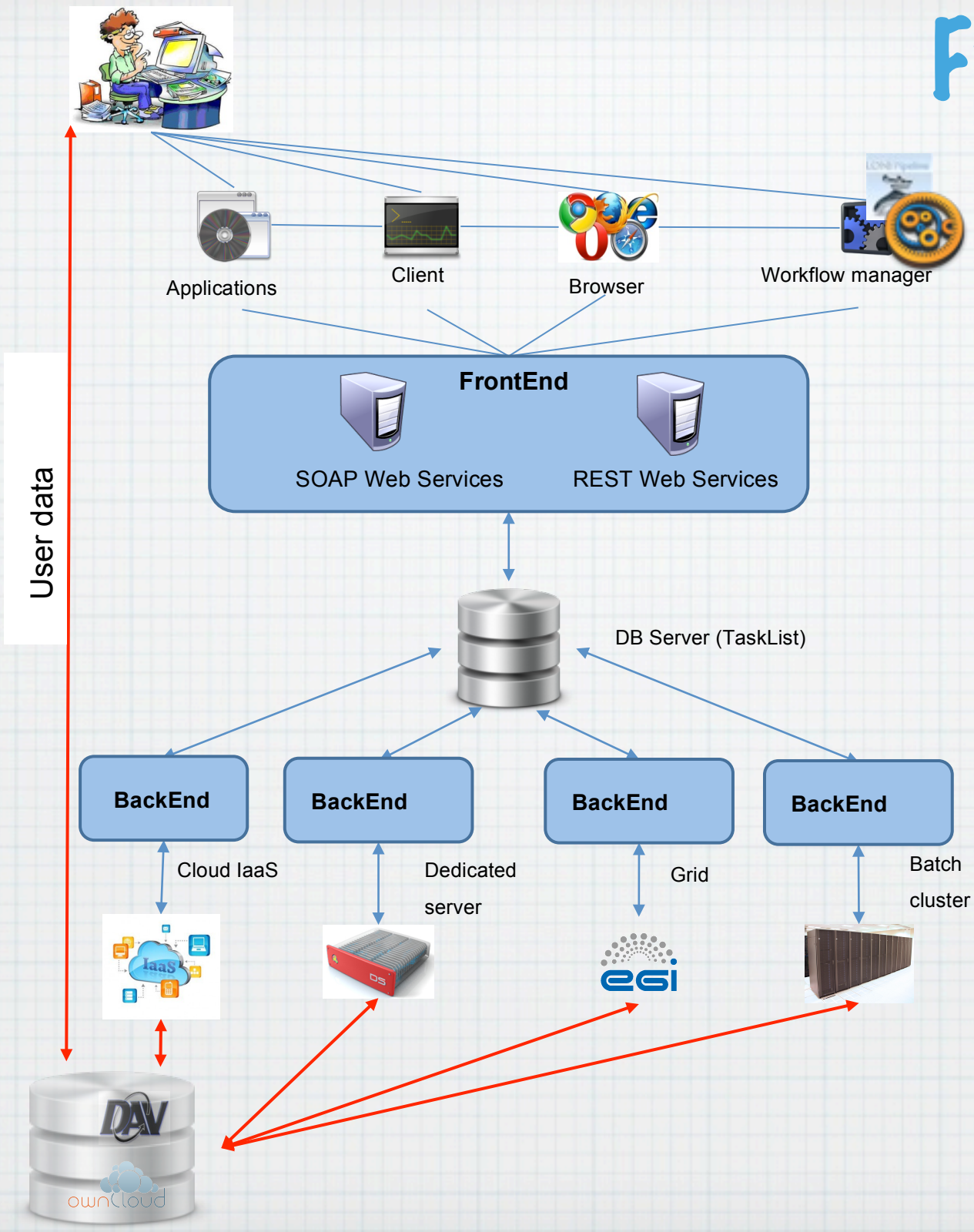


results: map showing the potential ecological niche of an African species re-using the same workflow --or an altered version of it-- as for the south east Asia horseshoe crab.

Status of the project

- We're at the second year of the project:
  - Several workflows available:
    - Public Shared: Data refinement, Population modelling, Ecol. niche modelling
    - Already available: Phylogenetic inferencing
    - In the pipe: Biogeochemical process modelling, metagenomics, ...
  - Using Web services from GBIF, CoL, CRIA, Fraunhofer, INFN, ...
    - Developing new services: viz and data selection, phylo, metagenomics, Biome-BGC modelling, pop modelling
  - A curated public catalogue of Web services
    - www.biodiversitycatalogue.org
  - AWS cloud infrastructure, new user interfaces (tavlite1.biovel.eu)
  - Growing profile in community
    - Steady enquiries from potential users and public training workshops

Framework Layout



General Overview of the Framework

- **FrontEnd**:
  - REST-FUL and Soap Web service
    - Apache TomCat
    - DBMS: MySql 5
    - Framework Jersey, Framework Java EE 6.0
    - SDK Asynchronous operations
  - It is able to deal with bunch operations (Submit & Check Status)
- **BACKEND** written in JAVA (Multithread)
  - Reads DB, submits jobs, executes tasks or instantiate a VM
  - At the moment we support:
    - PBS, EGI/IGI grid infrastructure, dedicated servers, Cloud infrastructures (**EC2**)
    - work in progress to support **SLURM**

General Overview of the Framework

- Each call to the web service is intended to request for an execution of a **well specified application**:
  - **Only supported applications** (and well known to the service provider) could be executed
  - Supporting a **new application** is usually **one day of works** from the service provider point of view
  - Most of the application is customized by one or few input files
    - The user can request a run, by choosing the **name of the application** and the **name** (and **location**) of the **input files**
    - You can also use a external file available through http, ftp, etc.
  - When needed, the user could change also parameters used in the command line
- The **output** of the runs, will be available (also to other services) via **http link**

Describing the application

- Each application is described by:
  - A **bash script** that prepare the environment and run the real application
    - Hidden to the final user
  - A set parameters
    - **Input location** and file name
    - **Arguments** for the executable
- Returns:
  - Status
  - **Output URL**

Describing the application

* Requesting execution of application for:
  * Huge challenges on distributed computing infrastructure (EGI)
    * >1000 jobs && >1 month of CPU
    * Response time: few days
  * Hundreds of parallel executions on a local batch farm (INFN-Bari--ReCaS)
    * Few hundreds-thousand of jobs
    * Response time: from few minutes to few hours
  * Fast execution (real time analysis) on a dedicated server
    * ~10 concurrent execution
    * Response time: ~ 5-10 seconds
    * Specialized HW: GPU, etc
  * Each of the application/service is already configured to run on a specific infrastructure

Job Submission Tool Features

* JST is a typical pilot job factory that is lightweight, multi-platform, and easy to use and maintain
* JST acts **on top** of the **Grid/Cloud middleware** so that users are not required to learn in details the technicalities of each infrastructure
* When the jobs reach the **execution host** they request to the **TaskListDB** if there is any task to execute (**pull mode**).
* JST tries to use all the computing resources available on the grid (no a priori black or white lists are strictly required). If the environment/configuration found on the WN is not adequate, the job exits.
* Since the **tasks are independent** and they can be resubmitted when failures occurs, good reliability can be reached and JST can work successfully even if some failure occurs on infrastructure services
  * We could use two or more instances for each critical service
    * i.e. Storage Element, RDBMS, front-end

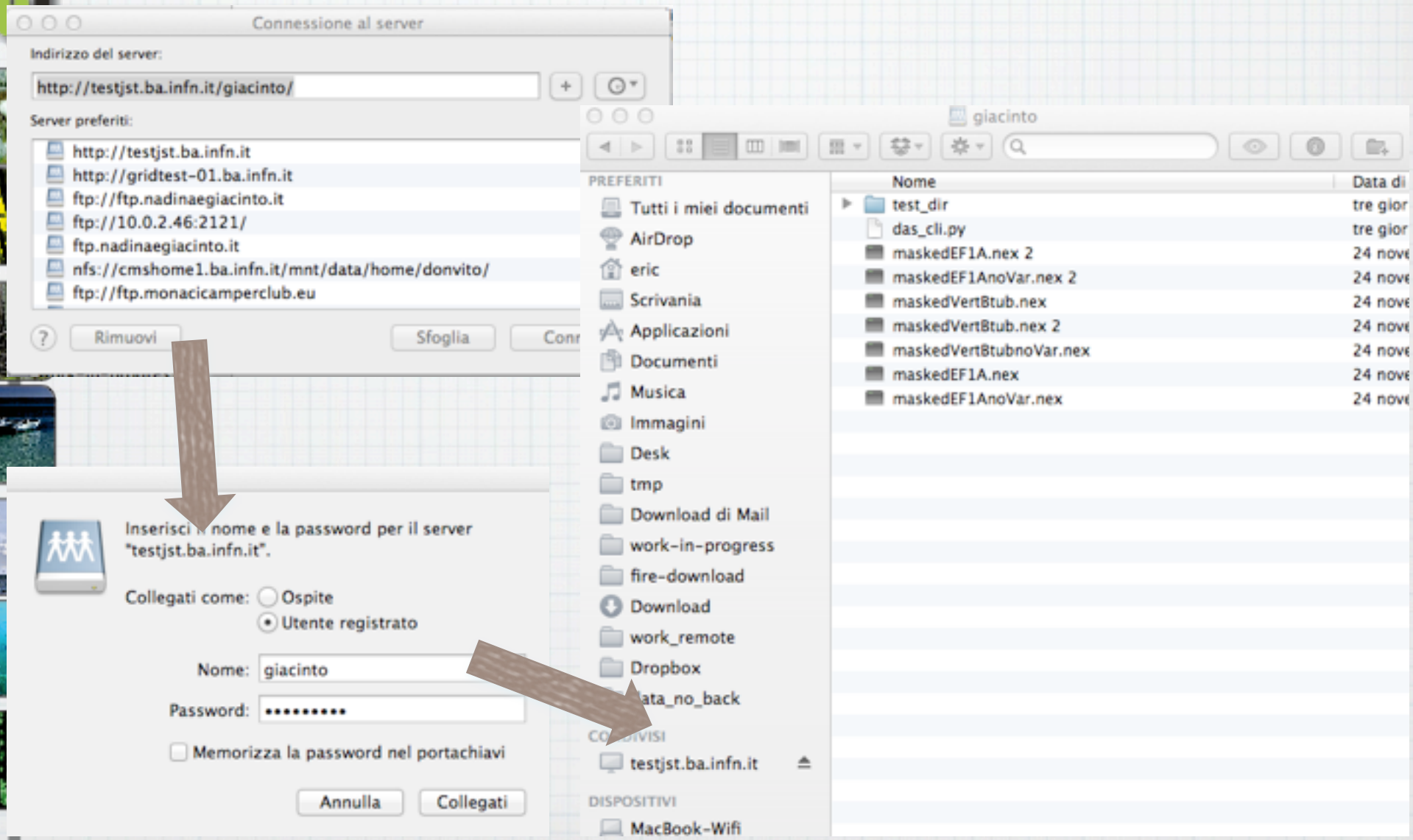
Job Submission Tool Wrapper

* **Requests from the TaskListDB** a tasks to be executed
* Retrieves the **application executable** and the **input files** (they has to be available with one protocol among: https, http, gridftp, ftp, xrootd)
* **Executes the application** code
* **Stores the output** in one of the configured SEs
  * With one of the configured protocols
* **Checks the exit status** of the executable and of the stage-out procedure
* **Updates the task status** into TaskListDB

Input file: problems and requirements

* Quite often the size of the **input files is O(GB)** so it is quite difficult to upload them using the standard web service interface
* Typical Bioinformatics **users do not know how to register input files into grid storage** elements and catalogues
* We need to provide an easy interface to **manage large files** and then transfer them to the grid in a transparent way
* This transfers service should:
  * Have at least one client in every platform (Windows/MacOS/Linux)
  * Provide authentication at least with username/password
  * Provide high performance on **high-latency networks**
  * **Reduce the file transfers** between services and users desktop to the minimum (**temporary files should be already available to the services**)

Screenshots: WebDav Datamanagement Service

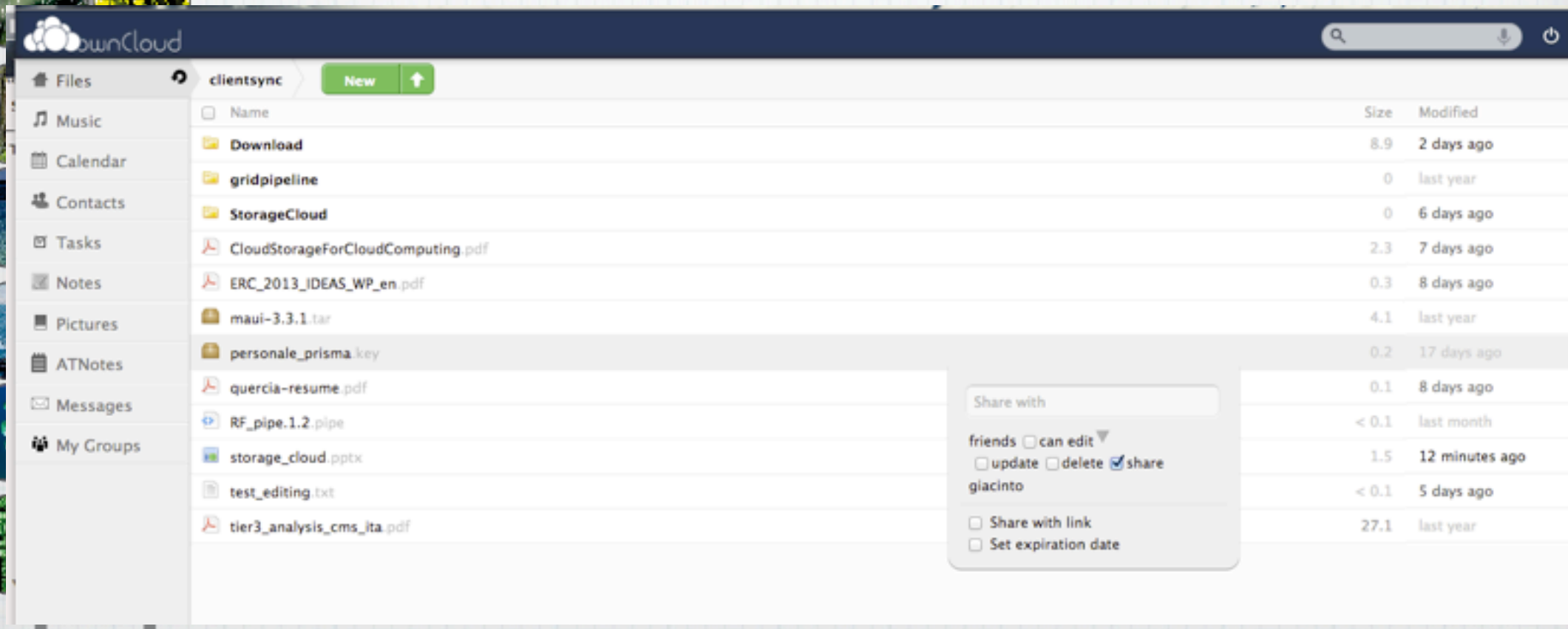


Screenshots: WebDav Datamanagement Service

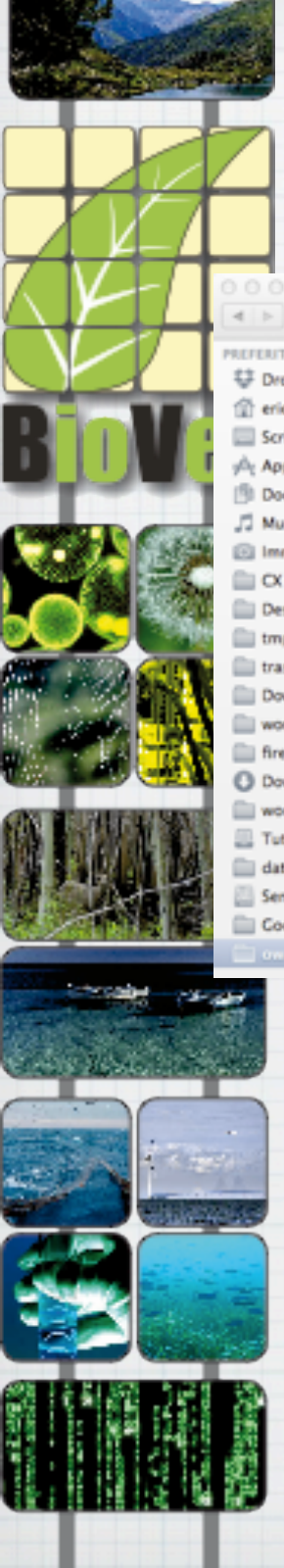
- You can access those files using web browser:
  - You can easily share your data with others colleagues
  - Or use the input/output within other (web) services

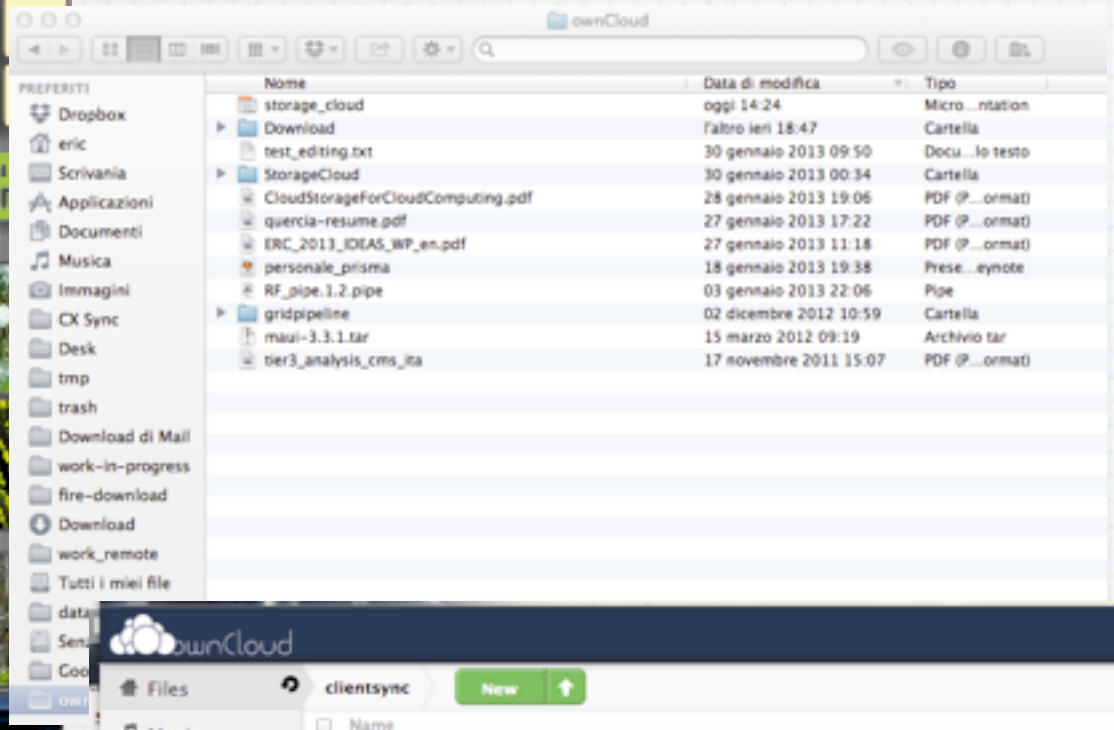
Screenshots: ownCloud Datamanagement Service

* It is Open Source and you can install in your hardware infrastructure
* It has both desktop client for synchronization, web and WebDav interface

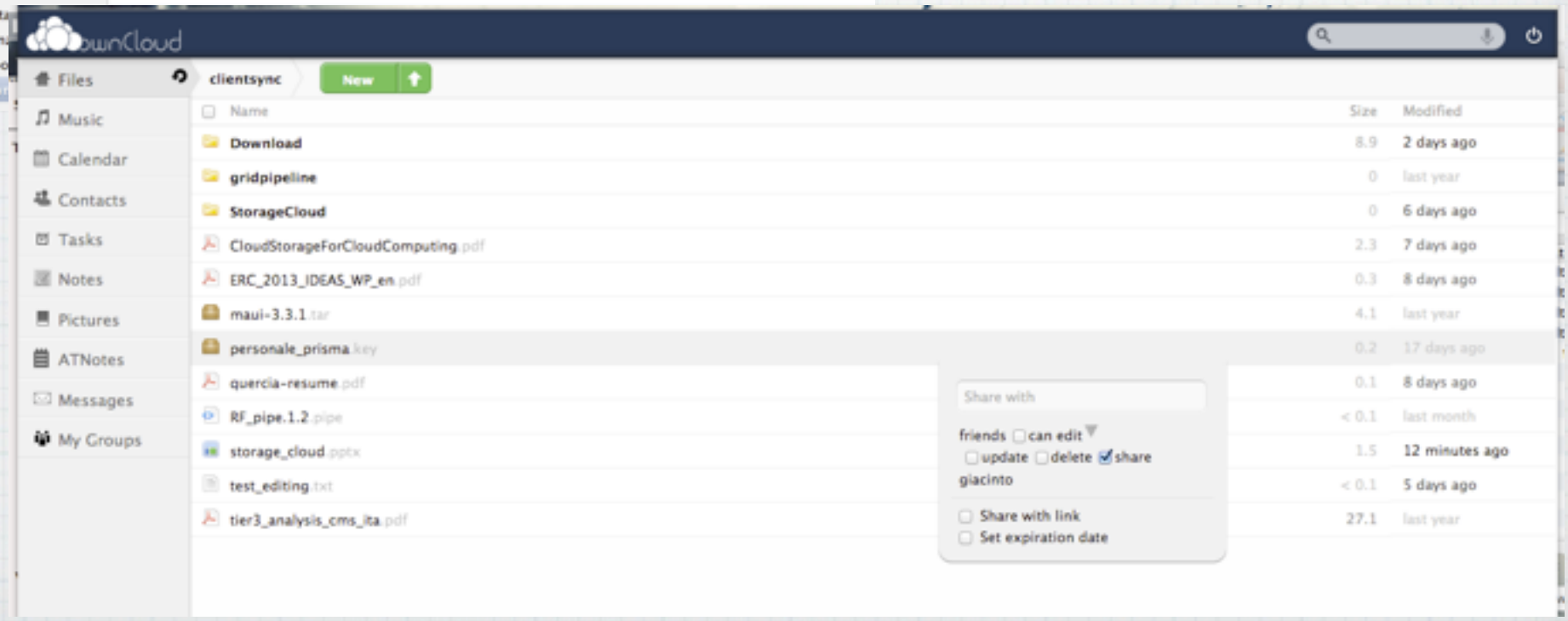


Screenshots: ownCloud Datamanagement Service

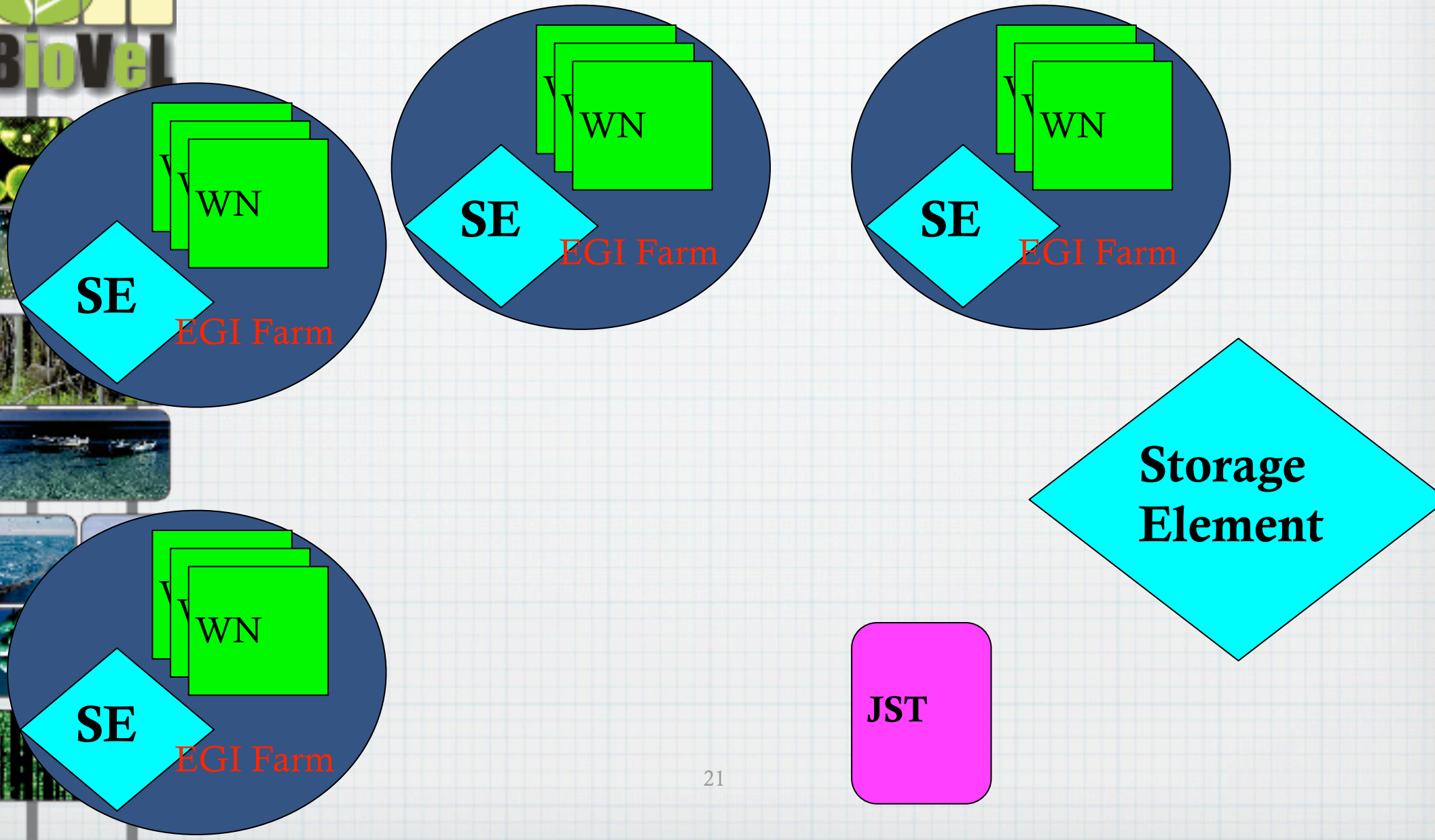




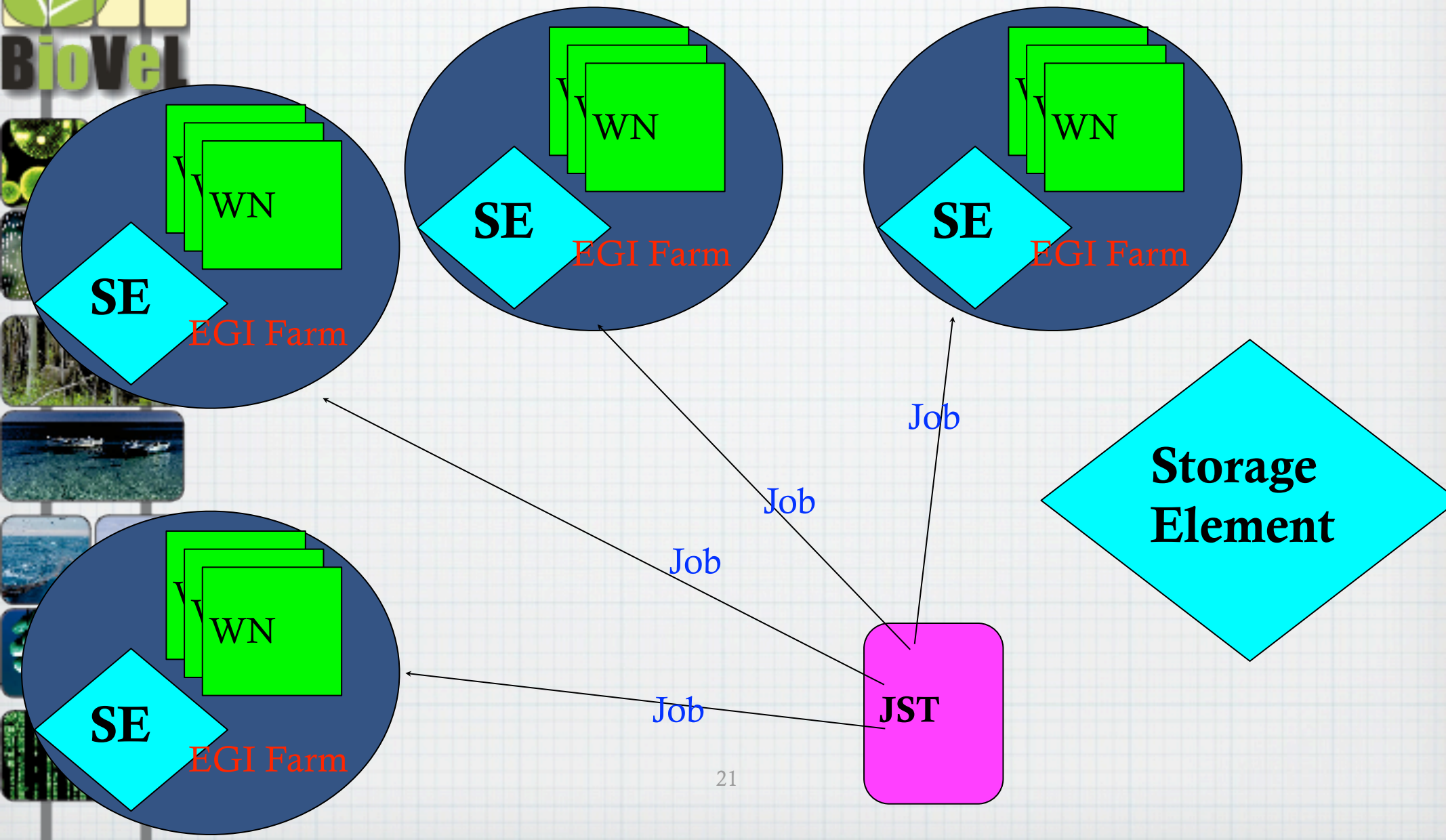
- A user could share files with other peoples & groups
- The end user could also create their own group of users



Data-Management and Bioinformatics applications over the Grid



Data-Management and Bioinformatics applications over the Grid



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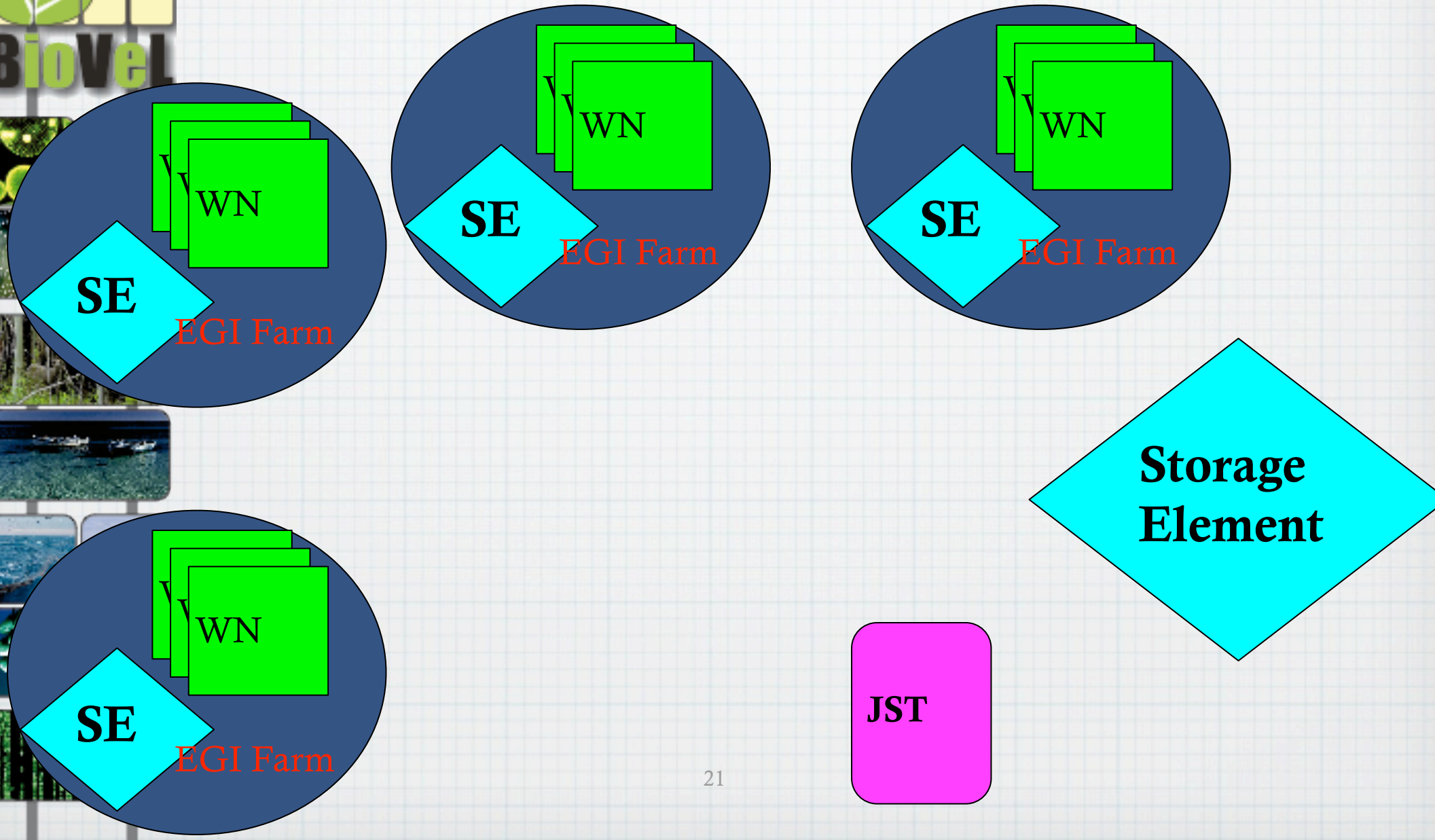

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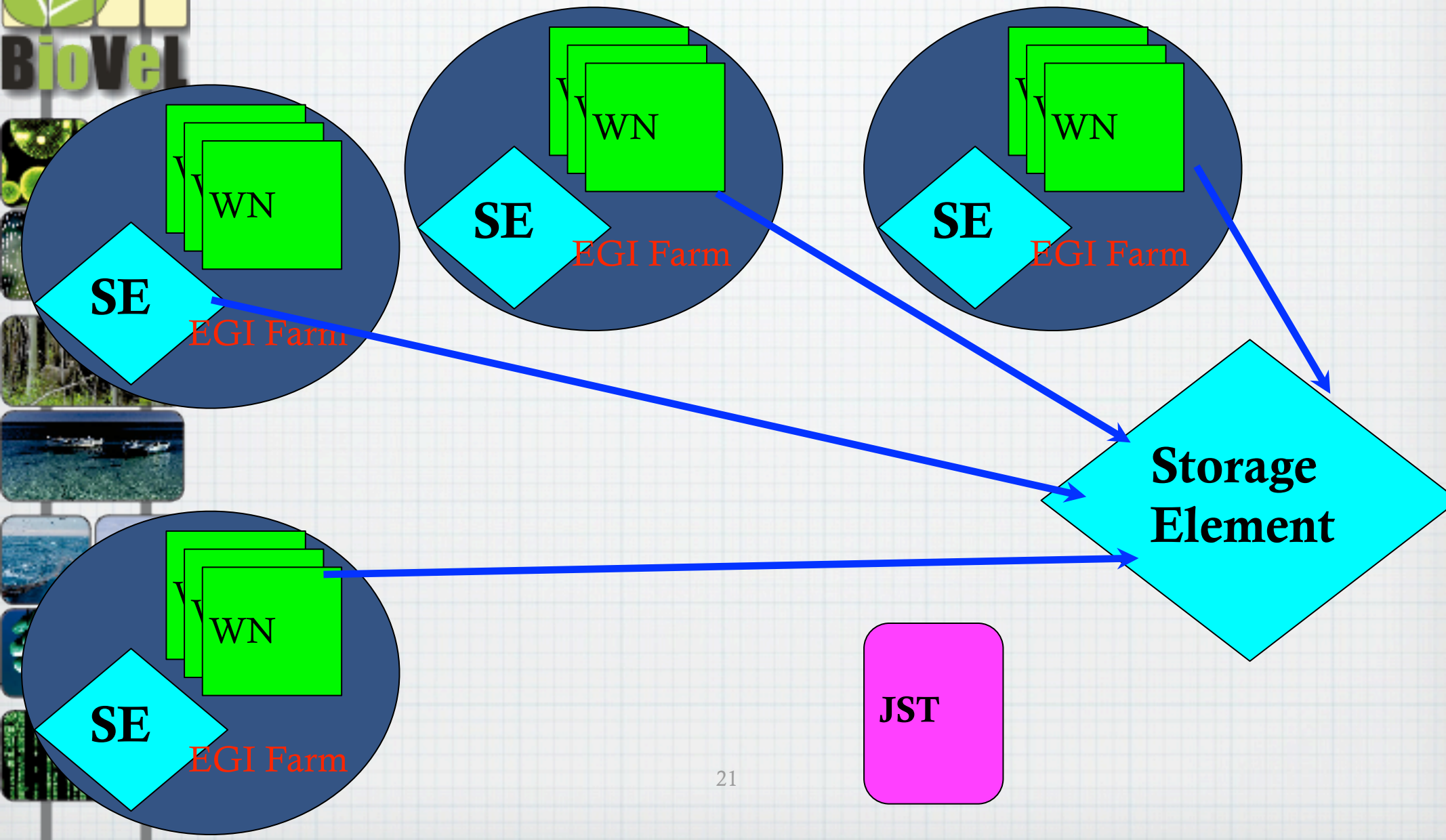

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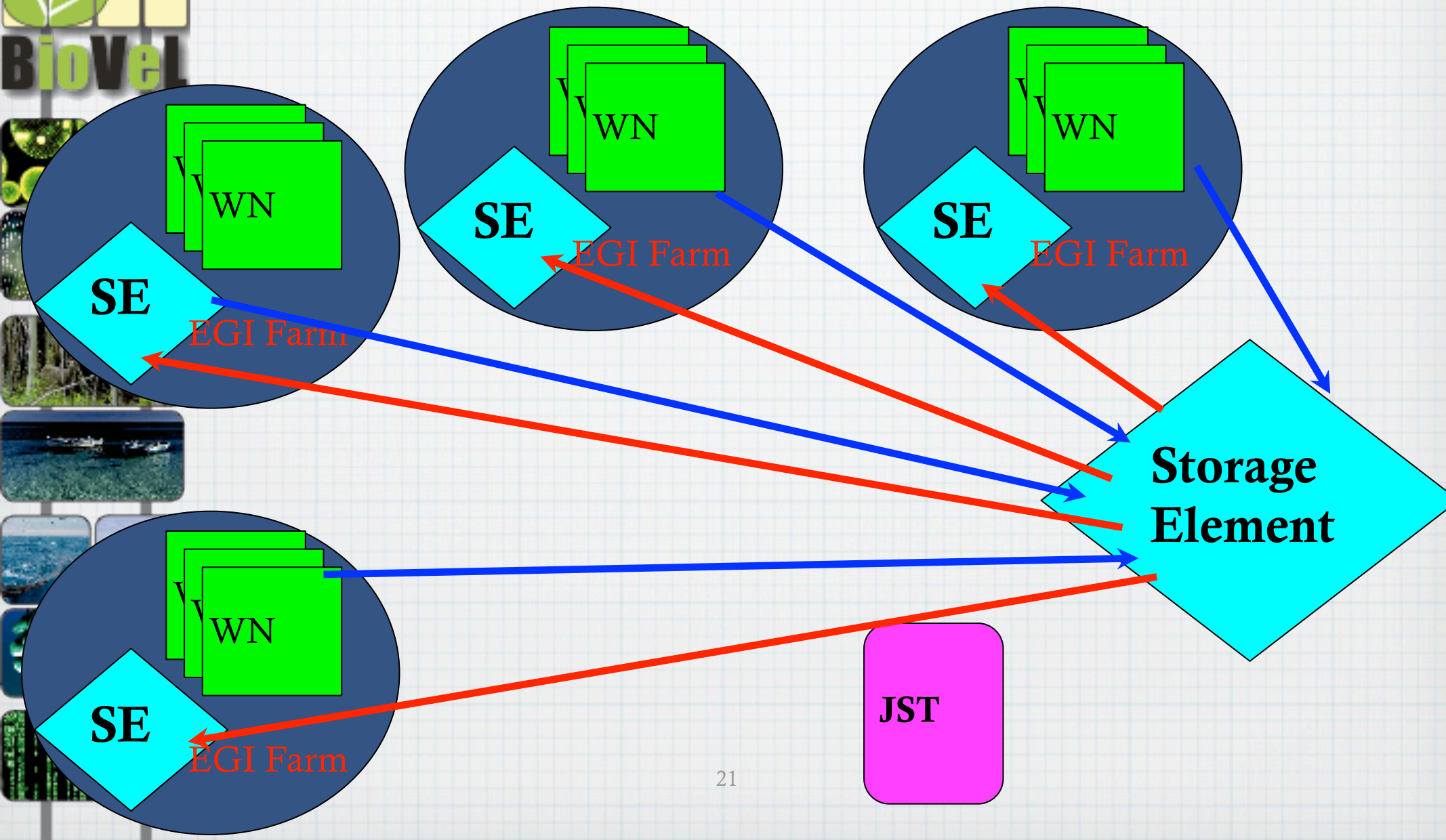

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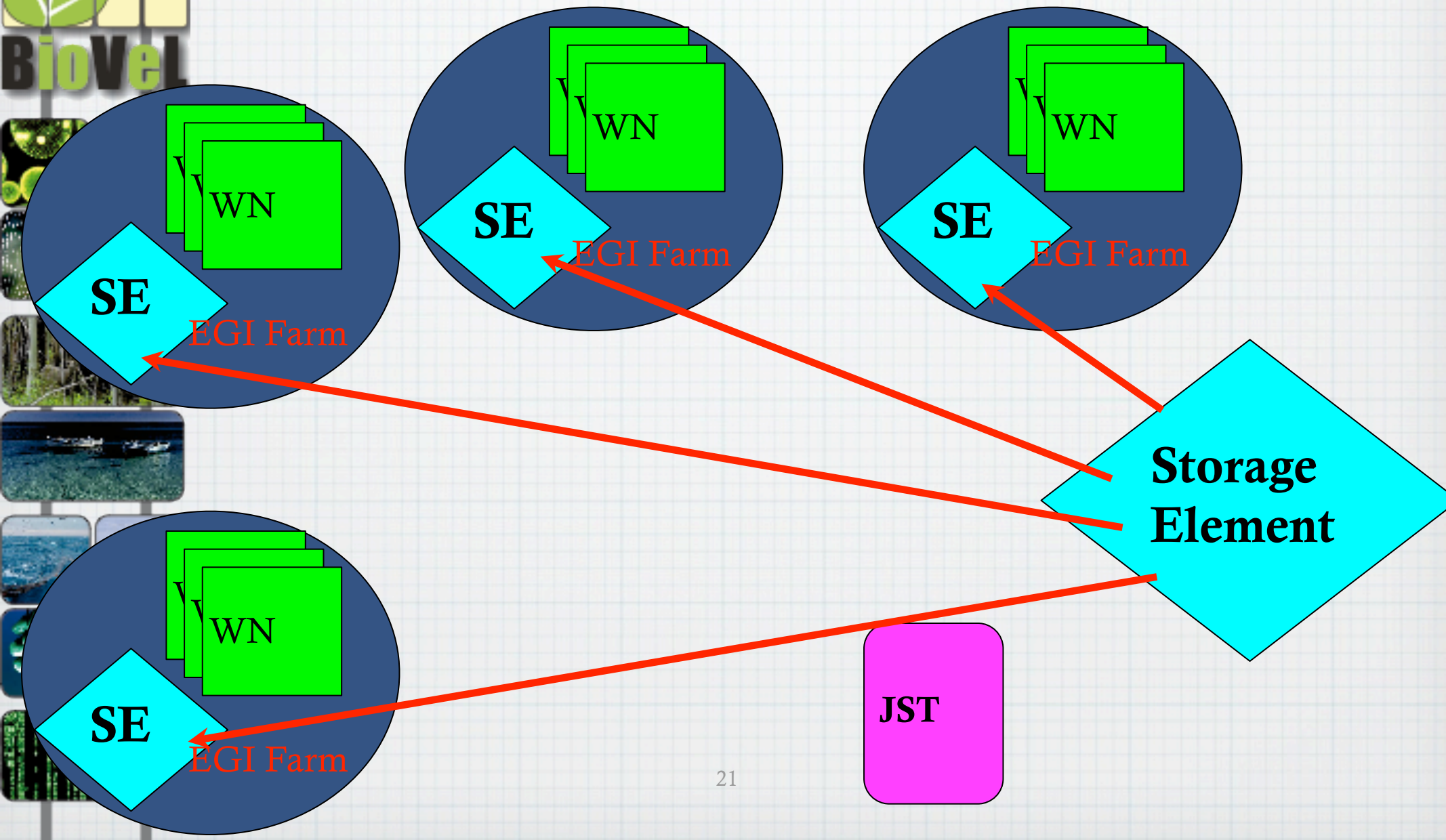

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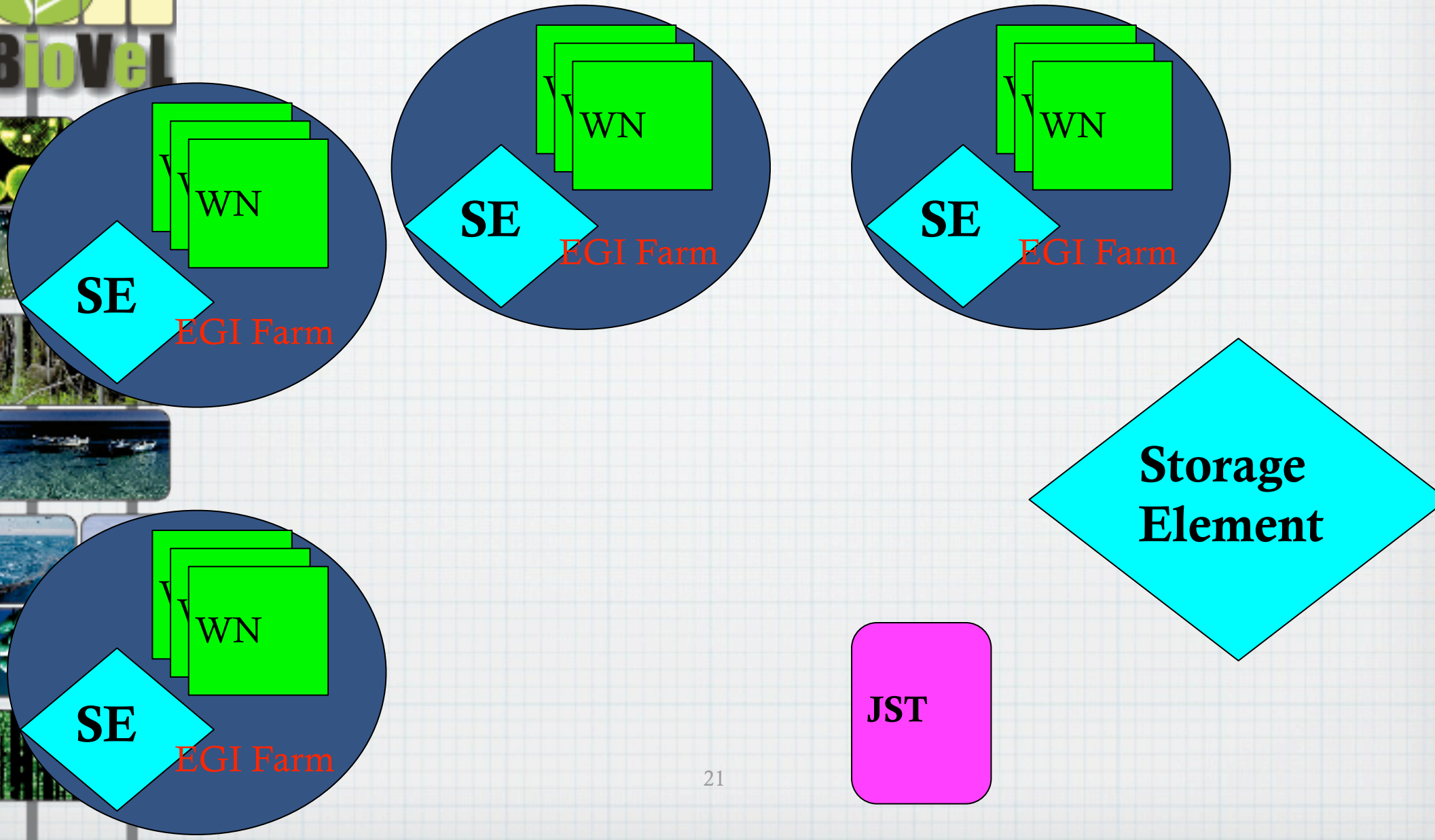

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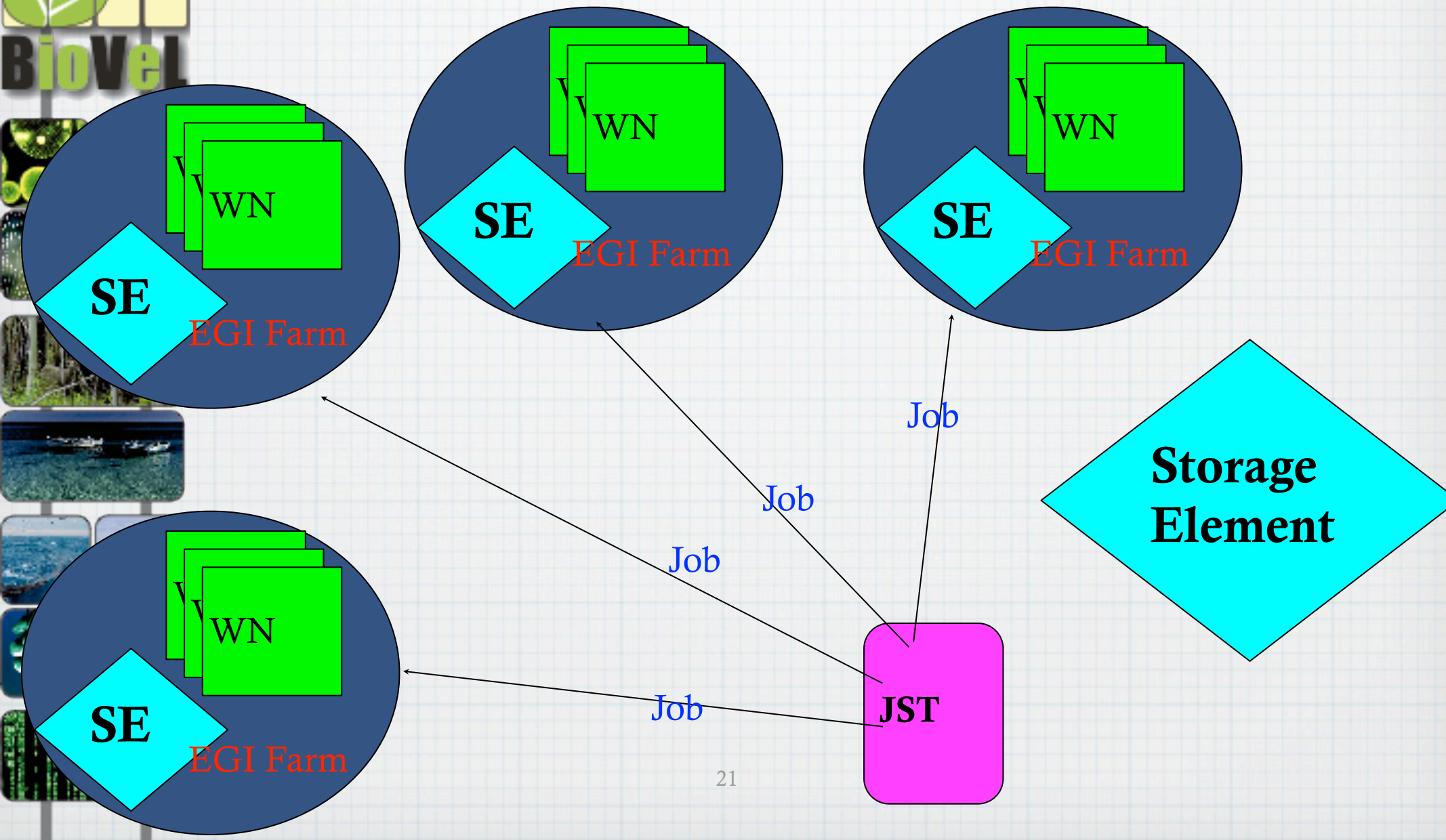

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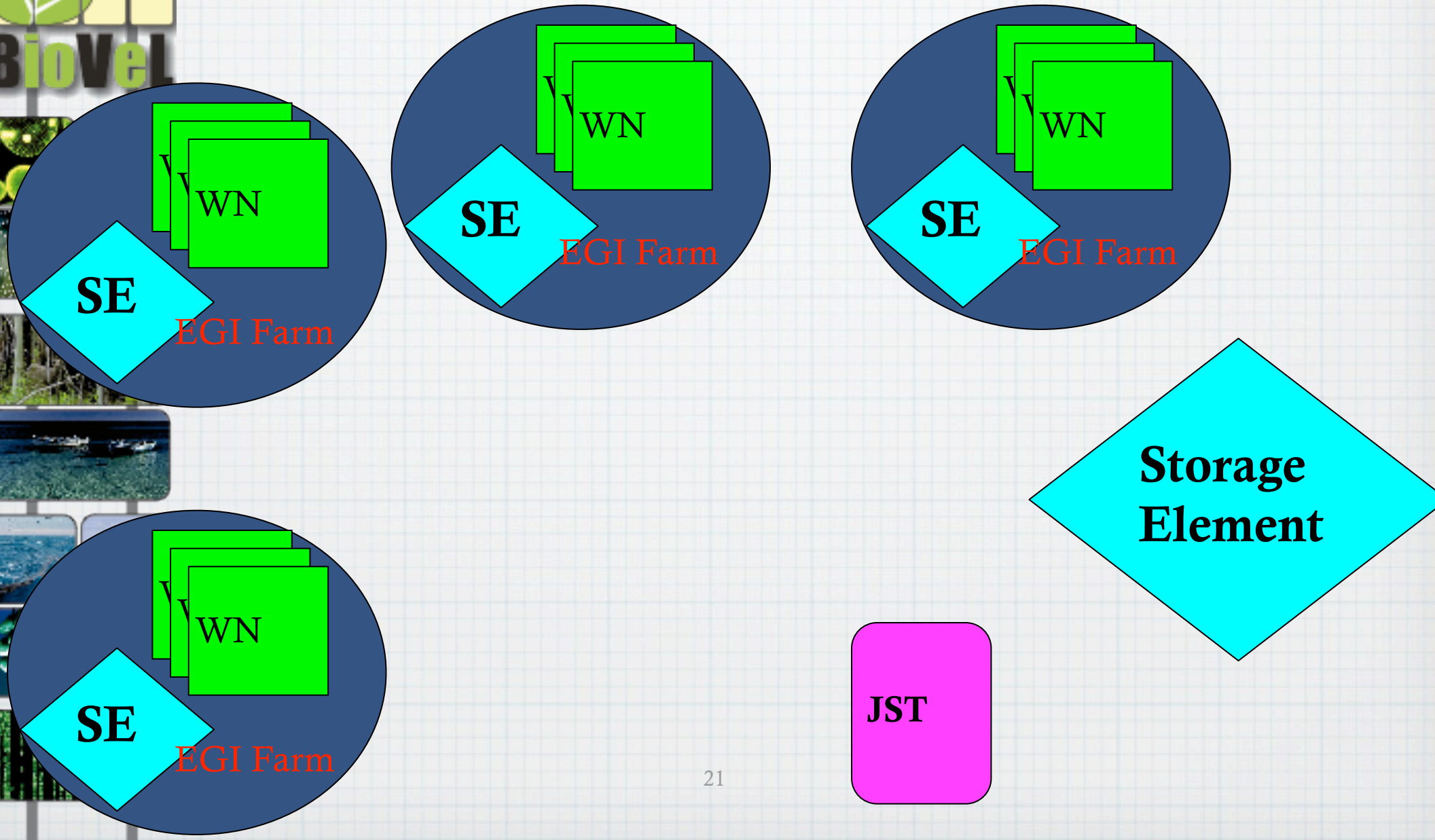

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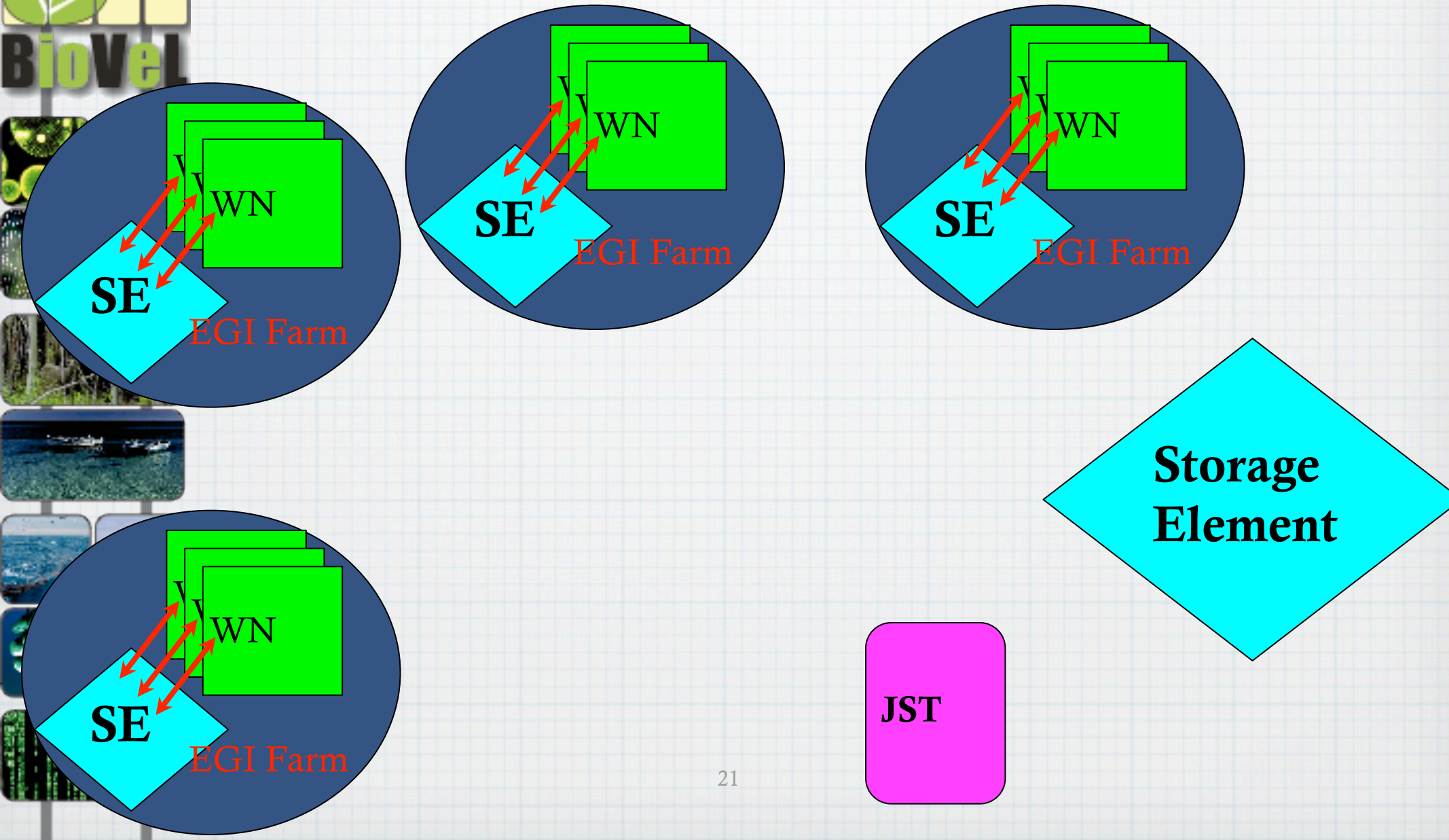


REST web services examples

* Insert Jobs:
  * http://localhost:8080/RestService/services/QueryJob/InsertJobs?NAME={blast}&arguments={http://webtest.ba.infn.it/vicario/FinalFusariumDB_2.nex ArgOne; http://webtest.ba.infn.it/vicario/FinalFusariumDB_1.nex ArgTwo;}


```
▼<Job>
  <Name>blast</Name>
  <Flag>f1966c8a-e926-4d17-a08a-4f83654d57ce</Flag>
 ▼<JobsID>
    <JobId>453112</JobId>
    <JobId>453113</JobId>
  </JobsID>
</Job>
```

REST web services examples

* Select Jobs:
  * http://localhost:8080/RestService/services/QueryJob/SelectJobs?FLAG={20b3cbf8-6805-47b4-ad7c-7b40bc706741}


```
▼<Jobs>
  ▼<Job>
    <Arguments>1</Arguments>
    <Comment>grid</Comment>
    <CPUs>1</CPUs>
    <Flag>f1966c8a-e926-4d17-a08a-4f83654d57ce</Flag>
    <Id>453112</Id>
    <LastCheck>2011-11-28 10:30:17.0</LastCheck>
    <Name>blast</Name>
    <Output/>
    <Provenance/>
    <Status>free</Status>
  </Job>
  ▼<Job>
    <Arguments>2</Arguments>
    <Comment>grid</Comment>
    <CPUs>1</CPUs>
    <Flag>f1966c8a-e926-4d17-a08a-4f83654d57ce</Flag>
    <Id>453113</Id>
    <LastCheck>2011-11-28 10:30:17.0</LastCheck>
    <Name>blast</Name>
    <Output/>
    <Provenance/>
    <Status>free</Status>
  </Job>
</Jobs>
```

SOAP Web Service examples

- wsdlpull 'http://localhost:8080/INFN.Grid.SoapFrontEnd/SoapServiceMethodsPort?wsdl' **InsertJobs** admin admin test_loni 'MatLabRUN1 input_test 12; MatLabRUN2 input_test2 24' pasq.notra@ba.infn.it

```
return:
Name:test_loni
Flag:f96ff248-d63a-4752-ae56-50ec088c97d4
JobsID:
JobId:454740
JobId:454741
```

- wsdlpull 'http://localhost:8080/INFN.Grid.SoapFrontEnd/SoapServiceMethodsPort?wsdl' **SelectJobs** admin admin 20b3cbf8-6805-47b4-ad7c-7b40bc706741

Tests and results

- Stress test already passed:
  - 100'000 insert in a loop... no memory leak or similar problems
  - Up to 100 concurrent clients without problems
  - 1000 tasks insert in a single REST call
  - ~1M of tasks managed from DB+backend
  - several public demos already executed
- A lot of experience in porting Bioinformatics application over EGI distributed computing infrastructure:
  - Hmmer, MrBayes, Blast, PAML, MUSCLE, EMBOSS, Biopython, AmpliconNoise, ABCtool, Bowtie, BayeSSC, GeoKS, hyphy, raxmlHPC, phylocom, consensus_xml, Matlab, etc...
- 30 different services already provided to users communities

Tests and results

* We already test the framework with two different workflow manager **LONI Pipeline** and **Taverna**
  * Also Taverna Lite is tested and it works perfectly
* But also simple command line could be used successfully:
  * **curl** -> REST web services
  * **wsdlpull** -> SOAP web services
* The "Dedicated Execution host" could be deployed in a generic **IaaS cloud solution**
  * test are already carried on successfully with **Amazon**, **OpenStack** and Proxmox
* All the "central services" could be easily deployed using a Cloud Infrastructure in order to easily achieve **High Availability**

Upload the user's inputs

Run MrBayes: a MPI application that could run for several hours

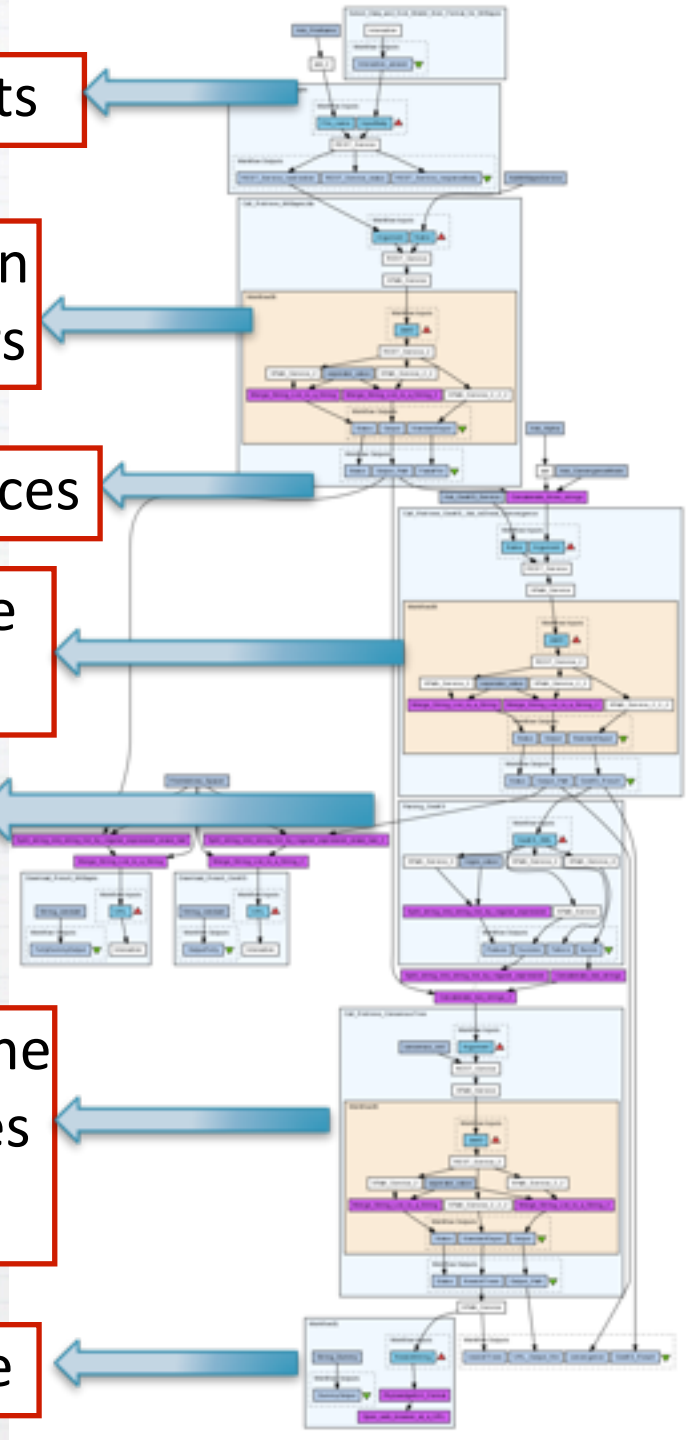
Pass the output to the next services

Check the convergence of the model

Retrieving the output and parsing the XML

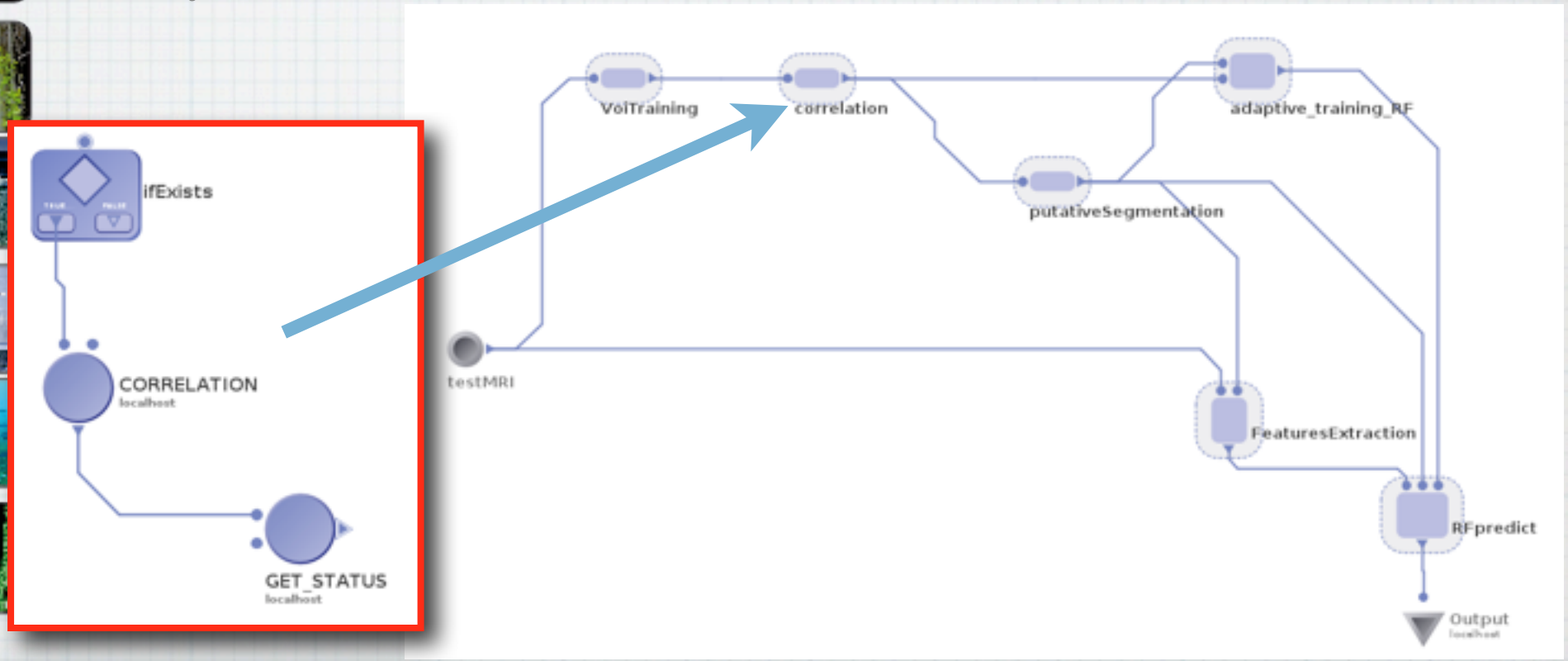
calculate the consensus tree of the posterior distribution of MrBayes output

Graphical view of the tree



LONI Pipeline

* GOAL: Analysis of neuro-images to diagnose the Alzheimer disease
* Several different libraries/application used:
  * Matlab, ITK, etc
* LONI Pipeline used to orchestrate the complex analysis workflow
* The analysis chain is quite long in terms of number of different programs to be executed



www.biodiversitycatalogue.org

A fully curated, well-founded catalogue of Web services for biodiversity science

BiodiversityCatalogue
"The Biodiversity Sciences Web Services Registry"

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catalogue of life | computation | darwincore | data upload | ecology | gbif | interpolation | modelling | MrBayes | MultiCPU | occurrence | raster | registry | shim | taverna | taxon | visualization | webclient | woa | workflows

Filtering

Current Filters Applied

none

Select filters from below...

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Service Types (2)

- REST (11)
- SOAP (3)

Service Categories (53)

- Taxonomy (5)
- Analysis (3)
- Modelling (4)
- Geospatial (1)
- Data (2)
- Visualization (3)
- Publishing (1)
- Ships (1)

Displaying **all 14** services | Include archived services? | Sort by: Newest | View: Grid

openModeller SOAP
Categories: Niche Modelling (Species Distribution)
Functionally equivalent to the openModeller service provided by modeller-cria-org-br, this endpoint is located in Eur...
Provider: omws-i3m-upv-es

BGBM CDM Cat ... ife REST API REST
Categories: Taxonomy, Taxonomic Synonym Resolution, Taxonomic Diversity, Checklist and Classification
This web service namespace is an add-on to the already existing CDM REST API and provides information relating to sci...
Provider: BGBM EDIT

MrBayes 16 CPUs REST
Categories: none — Help categorise this...
The service launch a bayesian phylogenetic inference with MrBayes 3.2 (http://mrbayes.sourceforge.net/) asking as inp...
Provider: alicegrid17-ba-infn-it

MrBayes_16CPUs REST
Categories: Tree Inference
The service launch a bayesian phylogenetic inference with MrBayes 3.2 (http://mrbayes.sourceforge.net/) asking as inp...
Provider: alicegrid17-ba-infn-it

(Test) Check ... okup Service REST
Categories: Taxonomic Name Resolution
Gets a single GBIF backbone taxon (nub usage) or null doing a fuzzy name & classification match.
Provider: api-gbif-org

(Test) Check ... ank Services REST
Categories: Taxonomy
Services related to name usages: a name usage is a usage of a scientific name according to one particular Checklist i...
Provider: api-gbif-org

Oxford Batch ... ation Engine REST

GBIF Portal Web Services REST

BioSTIF REST

www.myexperiment.org A repository for sharing workflows

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Group: BioVeL

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Group for sharing workflows relating to BioVeL - Biodiversity Virtual e-Laboratory - FP7-283359 BioVeL

For more information visit http://www.biovel.eu/

Created at: Saturday 06 August 2011 @ 15:38:58 (UTC)

Unique name: biovel

News

Owner

Alan Williams

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37 shared items

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Alex Hardisty

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Tags (3) | Announcements | Comments (0) |

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Owner

Alan Williams

48 members

37 shared items

1 announcements

New/Upload

Group | GO

Alex Hardisty

My Profile [edit]

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My History

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My Stuff

5 Friends | 3 Groups

Friends

apoigne

Tavema 2

Original Uploader

Cherianm

Project

BioVeL

Data Refinement Workflow (10)

View

Download (v10)

Created: 11/04/12 @ 10:08:25 | Last updated: 27/02/13 @ 22:06:01

Credits: Cherianm

License: Creative Commons Attribution-Share Alike 3.0 Unported License

The aim of the (Taxonomic) Data Refinement Workflow is to provide a streamlined workflow environment for preparing observational and specimen data sets for use in scientific analysis on the Taverna platform. The workflow has been designed in a way that, â€¢ accepts input data in a recognized format, but originating from various sources (e.g. services, local user data sets), â€¢ includes a number of graphical user interfaces to view and interact with the data, â€¢ the output of each part of th...

Rating: 4.5 / 5 (2 ratings) | Versions: 10 | Reviews: 0 | Comments: 0 | Citations: 0

Viewed: 134 times | Downloaded: 49 times

Tags (24):

data quality and filtering | geo-temporal data selection and filtering | historical analysis | occurrence retrieval | spatio-temporal analysis | species distribution analysis | species occurrence | species richness and diversity | synonym expansion | taxonomic data cleaning and refinement | taxonomic name resolution | taxonomy

Taverna Interaction Service

Original Uploader

Vhernand

BioSTIF Example with more than 1 datasourc... (3)

View

Download (v3)

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Credits: Vhernand

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BioSTIF can be opened with more than one data sources. The example files are very large and need some time for loading Example of inputs for 2 data sources: contentTypes: a list of 2 values, each containing csv csvDataURIs: a list with 2 values: http://ww2.bgbm.org/temp/bioveli/pot_invasive_dc_output.txt http://ww2.bgbm.org/temp/bioveli/dc_37000_output.txt The user can filter or select data on BioSTIF and the urls with the result data are returned to the workflow.

Rating: 0.0 / 5 (0 ratings) | Versions: 3 | Reviews: 0 | Comments: 0 | Citations: 0

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Retrieve Phylogenetic inference with MrBay... (3)

View

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Created: 20/02/13 @ 13:42:45 | Last updated: 25/03/13 @ 16:31:47

Credits: Vicarios Giacinto Donvito Bachirb

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Retrieve Phylogenetic inference with MrBayes and test of MCMC convergence (GEOKS) and fit of the model on the data (Posterior Predictive test)

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Tags (24):

data quality and filtering | geo-temporal data selection and filtering | historical analysis | occurrence retrieval | spatio-temporal analysis | species distribution analysis | species occurrence | species richness and diversity | synonym expansion | taxonomic data cleaning and refinement | taxonomic name resolution | taxonomy

Taverna Interaction Service

BioSTIF Example with more than 1 datasourc... (3)

View

www.myexperiment.org A repository for sharing workflows

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Data Refinement Workflow (10)

View
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Created: 11/04/12 @ 10:08:25 | **Last updated:** 27/02/13 @ 22:06:01

Credits: Cherianm

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The aim of the (Taxonomic) Data Refinement Workflow is to provide a streamlined workflow environment for preparing observational and specimen data sets for use in scientific analysis on the Taverna platform. The workflow has been designed in a way that, â€¢ accepts input data in a recognized format, but originating from various sources (e.g. services, local user data sets), â€¢ includes a number of graphical user interfaces to view and interact with the data, â€¢ the output of each part of th...

Rating: 4.5 / 5 (2 ratings) | **Versions:** 10 | **Reviews:** 0 | **Comments:** 0 | **Citations:** 0

Viewed: 134 times | **Downloaded:** 49 times

Tags (24):

data quality and filtering | geo-temporal data selection and filtering | historical analysis | occurrence retrieval | spatio-temporal analysis | species distribution analysis | species occurrence | species richness and diversity | synonym expansion | taxonomic data cleaning and refinement | taxonomic name resolution | taxonomy

Taverna Interaction Service
Original Uploader
Vhernand

BioSTIF Example with more than 1 datasourc... (3)

View
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Created: 20/04/12 @ 15:01:25 | **Last updated:** 15/02/13 @ 14:33:10

Credits: Vhernand

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BioSTIF can be opened with more than one data sources. The example files are very large and need some time for loading Example of inputs for 2 data sources: contentTypes: a list of 2 values, each containing csv csvDataURIs: a list with 2 values: http://ww2.bgbm.org/temp/bioveli/pot_invasive_dc_output.txt http://ww2.bgbm.org/temp/bioveli/dc_37000_output.txt The user can filter or select data on BioSTIF and the urls with the result data are returned to the workflow.

Rating: 0.0 / 5 (0 ratings) | **Versions:** 3 | **Reviews:** 0 | **Comments:** 0 | **Citations:** 0

Viewed: 13 times | **Downloaded:** 13 times

This Workflow has no tags!

Taverna 2
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Retrieve Phylogenetic inference with MrBay... (3)

View
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Created: 20/02/13 @ 13:42:45 | **Last updated:** 25/03/13 @ 16:31:47

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Taverna Interaction Service

BioSTIF Example with more than 1 datasourc... (3)

View

Biodiversity Virtual e-Laboratory

BioVeL

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Workflow Entry: Show species distribution

Version 1 (of 1)

Title: Show species distribution

Type: Taverna 2

Preview

(Click on the image to get the full size)

Download Scalable Diagram (SVG)

Description

This workflow takes in the common name for an animal or plant and the start and end dates for observations. (It also needs the command to open Google Earth).

It uses the REST interface of the Integrated Taxonomic Information System to find the scientific names corresponding to the common name. The scientific names are extracted and sorted. The user is then able to select exactly which species is meant.

The workflow then uses the REST interface of the Global Biodiversity Information Facility to determine the location of observations. Those locations are accepted in KML format.

The KML data is then opened in Google Earth.

Workflow Type
Taverna 2

Original Uploader
Alan Williams

License

Credits (0)

Attributions (0)

Tags (7)
biodiversity | biovel | gbif | google earth | its | kml | nest

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BioVeL preliminary testing pack

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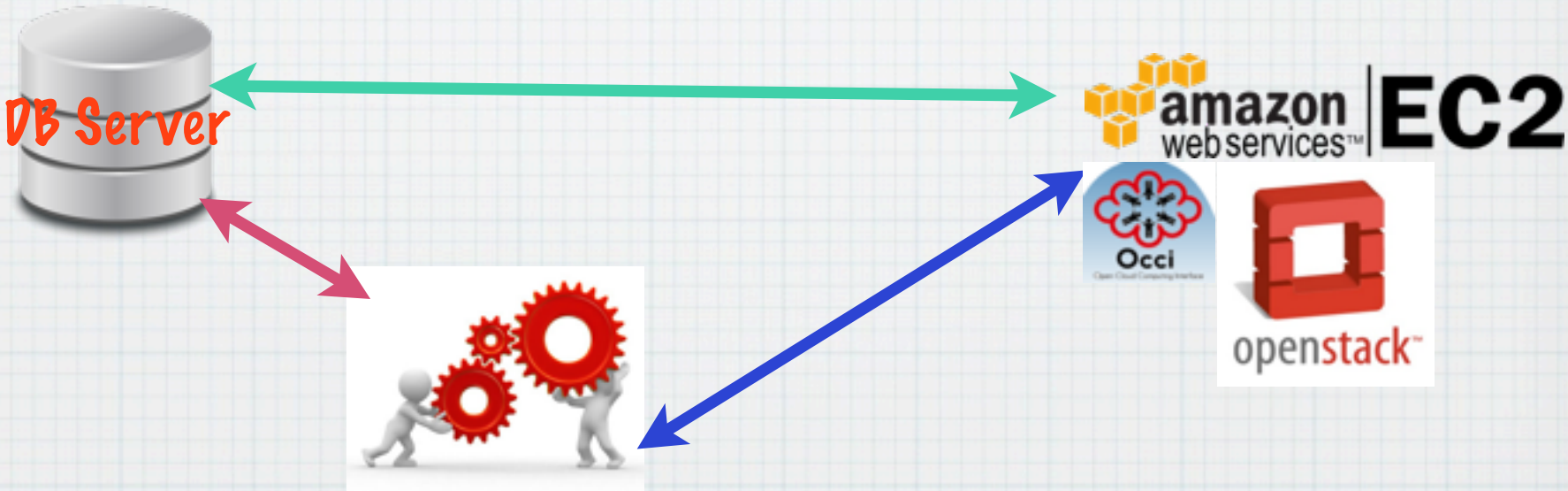
Popular Tags

Work-in-progress

* We are working to put all the JST components on the IaaS cloud infrastructure (both Amazon, OpenStack)
  * This will increase the HA capabilities
* We are developing an agent to ask for new working agent to the IaaS cloud (using EC2 and OCCI interfaces)



WM request agent

Conclusions & TO-DO

- We have a **high scalable** and **solid** service that could be used to supports execution of applications over **different computing infrastructure**
  - it provide a general enough solution that is already been used from two completely different communities to produce science and publications
    - biodiversity and biomedicine
    - using **Taverna** and **LONI Pipeline** workflow managers
- We have also a high performance data transfer and sharing service
  - with advance functionalities of desktop-server synchronization (Cloud Storage)

Conclusions & TO-DO

- We are able to exploit any kind of computing infrastructure:
  - standard server, local batch, grid, IaaS cloud
- We publish both services and WorkFlows on BioCatalogue and MyExperiments as soon as they are available
- It is quite easy to add new application as required from users
- simple procedure supported to configure the core services to provide high-availability
- We will soon add OpenID authentication, and SAML2
  - as soon as it will be required it would be easy to add GSI or Shibboleth security on the front-end

People involved

* Giacinto Donvito (INFN-Bari ReCaS)
* Pasquale Notarangelo (INFN-Bari)
* Saverio Vicario (CNR)
* Bachir Balech (CNR)
* Marica Antonacci (INFN-Bari)

Biodiversity Virtual e-Laboratory

BioVeL is funded by the European Commission 7th Framework Programme (FP7).
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Under FP7, the e-Infrastructures activity is part of the Research Infrastructures programme, funded under the FP7 'Capacities' Specific Programme. It focuses on the further development and evolution of the high-capacity and high-performance communication network (GÉANT), distributed computing infrastructures (grids and clouds), supercomputer infrastructures, simulation software, scientific data infrastructures, e-Science services as well as on the adoption of e-Infrastructures by user communities.

BioVeL is free and available via internet.

CAPACITIES

e-infrastructure

www.biovel.eu, contact Alex Hardisty: HardistyAR@cardiff.ac.uk