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Marine metagenomic infrastructure services as driver for research and industrial innovation

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WP6 Organization

- WP leaders:
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  - Rob Finn (EMBL-EBI)
- Participants:
  - Calouste Gulbenkian Foundation (Portugal)
  - CCMAR – Center for Marine Sciences (Portugal)
  - CNRS - The National Center for Scientific Research (France)
  - CNR - National Research Council (Italy)

Outline

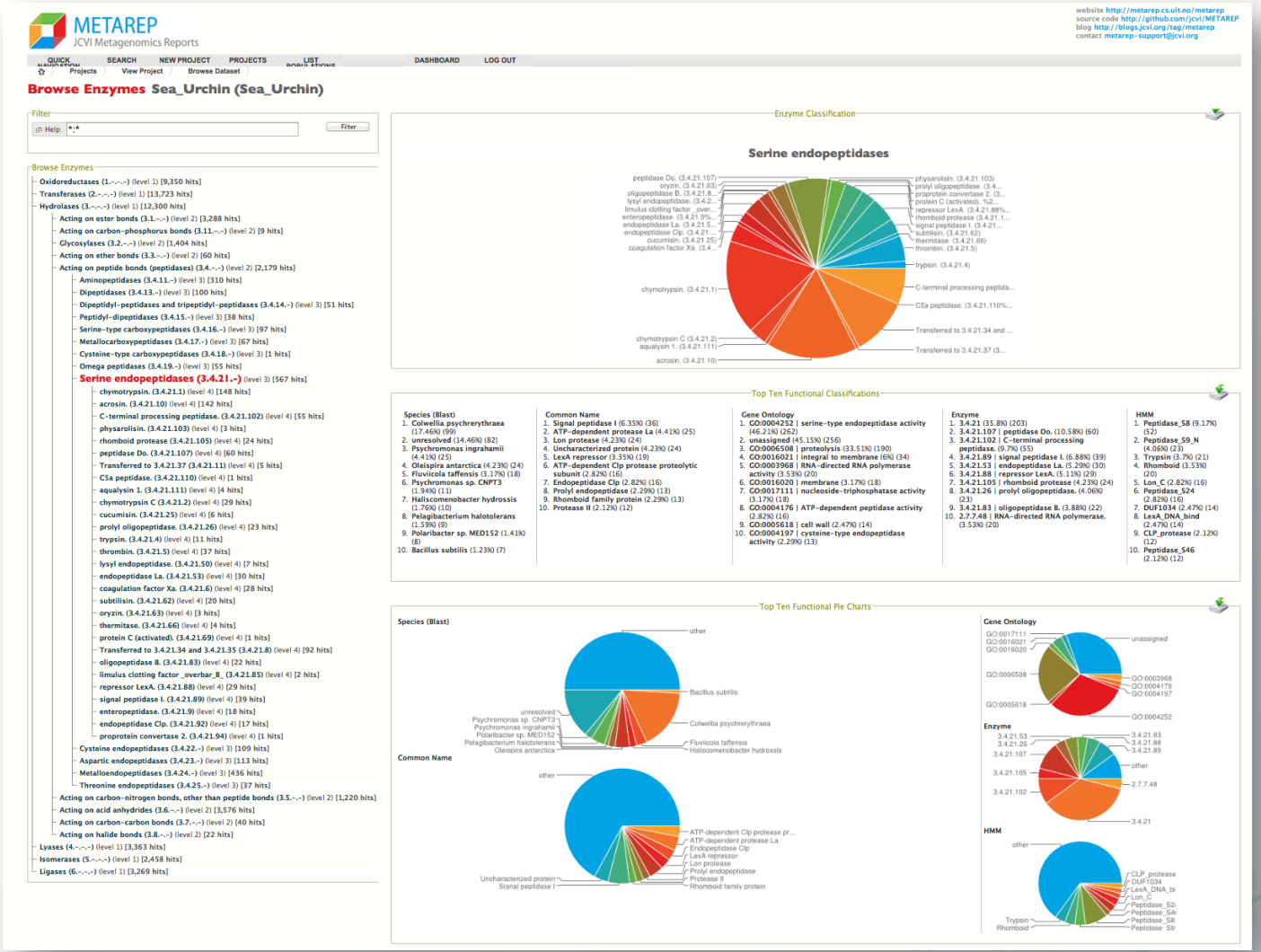
- Use case overview
  - Background
  - Pilot action
  - Use case
- Meta-pipe
  - Norwegian e-Infrastructure for Life Sciences (NeLS)
  - Galaxy/ supercomputer/ NeLS integration
- Technical workflow in use case

Metagenomics – Environmental Samples Analysis

Marine Metagenomics

- Marine genomics and metagenomics are rapidly expanding
- Need customized data, tools, pipelines, and analysis services for the marine domain

Cold Adapted Enzymes



Marine metagenomics pilot – towards domain specific service

- October 2014 – September 2015
- University of Tromsø and EMBL-EBI
- Start to harmonize our pipelines:
  - EBI Metagenomics Portal: generic metagenomics analysis pipeline
  - UiT META-pipe: marine metagenomics pipeline
- User community for marine metagenomics analysis in ELIXIR

Pilot Deliverables

- **Harmonize existing metagenomics pipelines to ensure interoperability**
- Assess new functionally specialized databases to enhance or enrich pipeline output
- Investigate the use of other approaches for taxonomic assignment, expanding beyond prokaryotic assignments
- **Explore and prototype with EBI Embassy Cloud**
- Report on gap analysis related to establishment of reference genomes for the marine environment
- Collaboration Workshop on Marine Informatics (16-17 March 2015)
- Report about the needs for specific investment in connection to services for the marine sector

Use case: Marine metagenomic infrastructure services as driver for research and industrial innovation

- Objectives:
  - Development and implementation of selected **standards** for the marine domain
  - Development and implementation of **databases** specific for the marine metagenomics
  - Evaluation and implementation of **tools and pipelines** for metagenomics analysis
  - Development of a **search engine** for interrogation of marine metagenomics datasets and establish training workshops for end users

Task 6.1: Data standards for marine domain

- Data format conventions and standards
- Reporting standards
- Validation tools

Task 6.2: Marine specific data resources

- Build high quality marine specific reference databases
  - Sequences from ENA, UniProt, and other datasets, including…
  - ...TaraOceans and Ocean Sampling Day
  - Collaboration with EMBRC and MIRRI

- TaraOceans: 15TB storage + 200 CPU years to calculate

Task 6.3: Gold standards for metagenomics analysis

- Evaluation and implementation of new tools and pipelines
  - Environmental applications
  - Results publically available
- Available through:
  - UiT META-pipe
  - EBI Metagenomics Portal (EBI MGP)
  - EMBL Embassy Cloud
  - …

Task 6.3: Gold standards for metagenomics analysis

- Web based search engine for interrogation of marine metagenomics results available from EBI MGP
  - Using existing web services
  - Discovery of data through metadata, taxonomic and functional fields
- Expanded comparison tool
  - User selected datasets
  - Functional and taxonomic comparison
  - Federated search over META-pipe and MGP results
  - Identification of common trends and/or differences

Task 6.4: Training workshops for end user

- Collaboration with ELIXIR Training Programme WP
- Exploit provided data, tools, pipelines, and compute infrastructures

META-Pipe

- Our marine metagenomics data analysis pipeline
- Elixir-NO delivery to Elixir
- Integrated with national infrastructure platforms
- Run on local supercomputer
- Deployed as national service

BETA

NeLS

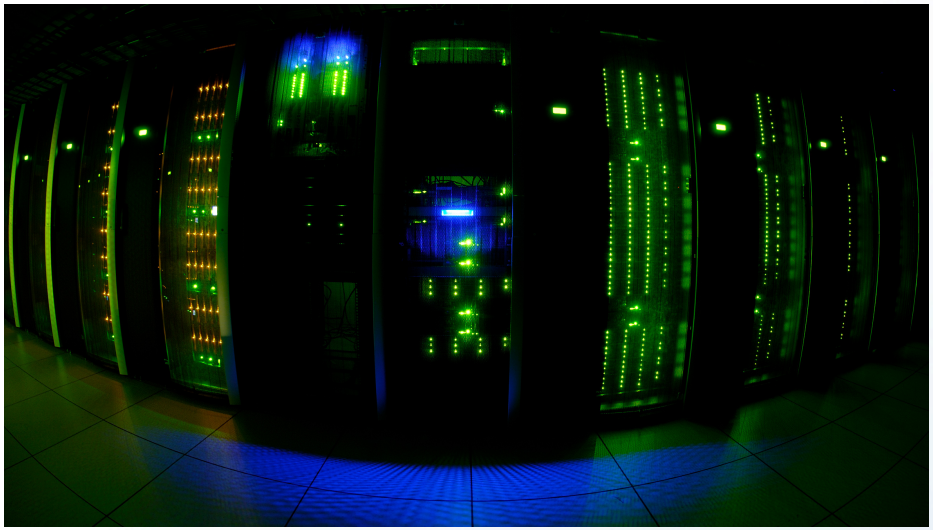
Norwegian e-Infratructure for Life Sciences

NeLS

- Galaxy as common GUI
- Federated login
  - Meta-pipe is accessible to all *FEIDE* users
  - Non-FEIDE users are special case
- Data sharing
  - META-pipe input and output data can be imported/exported to NeLS storage using Galaxy or scp
  - 40TB (soon 300TB) temporal storage for NeLS projects
  - Permanent storage in NorStore coordinated by StoreBioInfo

Stallo Supercomputer (UiT)

- 750 nodes, 14.000 cores
- 12.8 TB DRAM
- 2.1 PB of total disk capacity (1PB shared temporary storage)
- Centralized storage via Infiniband
- PBS/Torque



notur

norstore

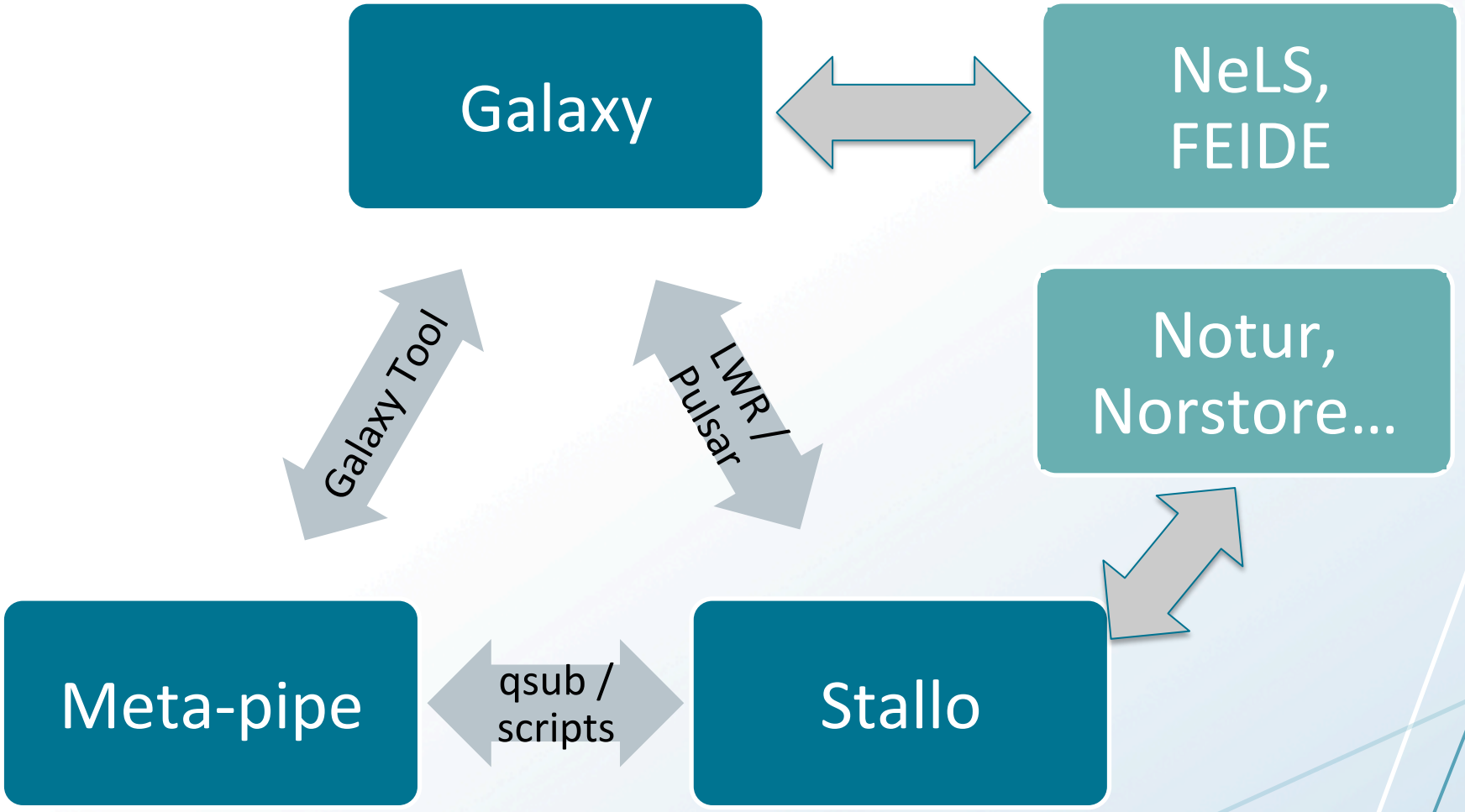
nhpc

PRACE

EUDAT

egi

Integration



Summary – Who are the stakeholders?

- Users:
  - Local, national, European, and international (accounting)
  - Academic and commercial (licenses)
- Service providers:
  - Pipelines hosted at EBI and UiT
  - Search engine hosted at EBI?
  - Marine resources databases hosted at?
- Resource providers:
  - EBI and UiT has resources for executing pipelines and searches
  - …storage resources in next slide
- Other stakeholders:
  - Other big EU projects: EMBRC and MIRRI

Summary – Where is the data?

- (Raw input data at individual labs)
- Example 1, EBI MGP:
  - Submit data to ENA
  - Analysis run at EBI
  - Results stored at EBI
- Example 2, META-pipe (Norwegian users):
  - Live data stored at Supercomputer
  - Temporary storage on NeLS storage systems
  - Permanent storage on national storage system
- Future:
  - Archival services and databases (ENA, UniProt)
  - Mirroring of MGP and META-pipe data for federated search?
  - Marine resources database at?
  - Search engine data?
  - Embassy cloud?

Summary – How big is the data? What are our computational needs?

- Estimate to use at least 0.5PB of disk
- We are optimizing our pipelines
- META-pipe:
  - UiT Supercomputer group not worried about resource usage
  - Pipeline scales with regards #users

Summary – How do we plan to manage data?

- Examples:
  - EBI MGP
  - META-pipe
  - Pilot project (harmonize results)

Summary – How do our users use the data?

- EBI MGP is a web application
- META-pipe is integrated with Galaxy
  - Will implement a web application interface for META-pipe
- Search engine will likely be a web application
- Also_ REST APIs and direct access to files

Summary

- Marine metagenomics
  - Pilot action
  - Use case
- Meta-pipe
  - Deployed as national service
  - Galaxy GUI
  - Integrated with local supercomputer
  - National storage resources (NeLS)
  - Federated login (NeLS)

Ongoing Work and Challenges

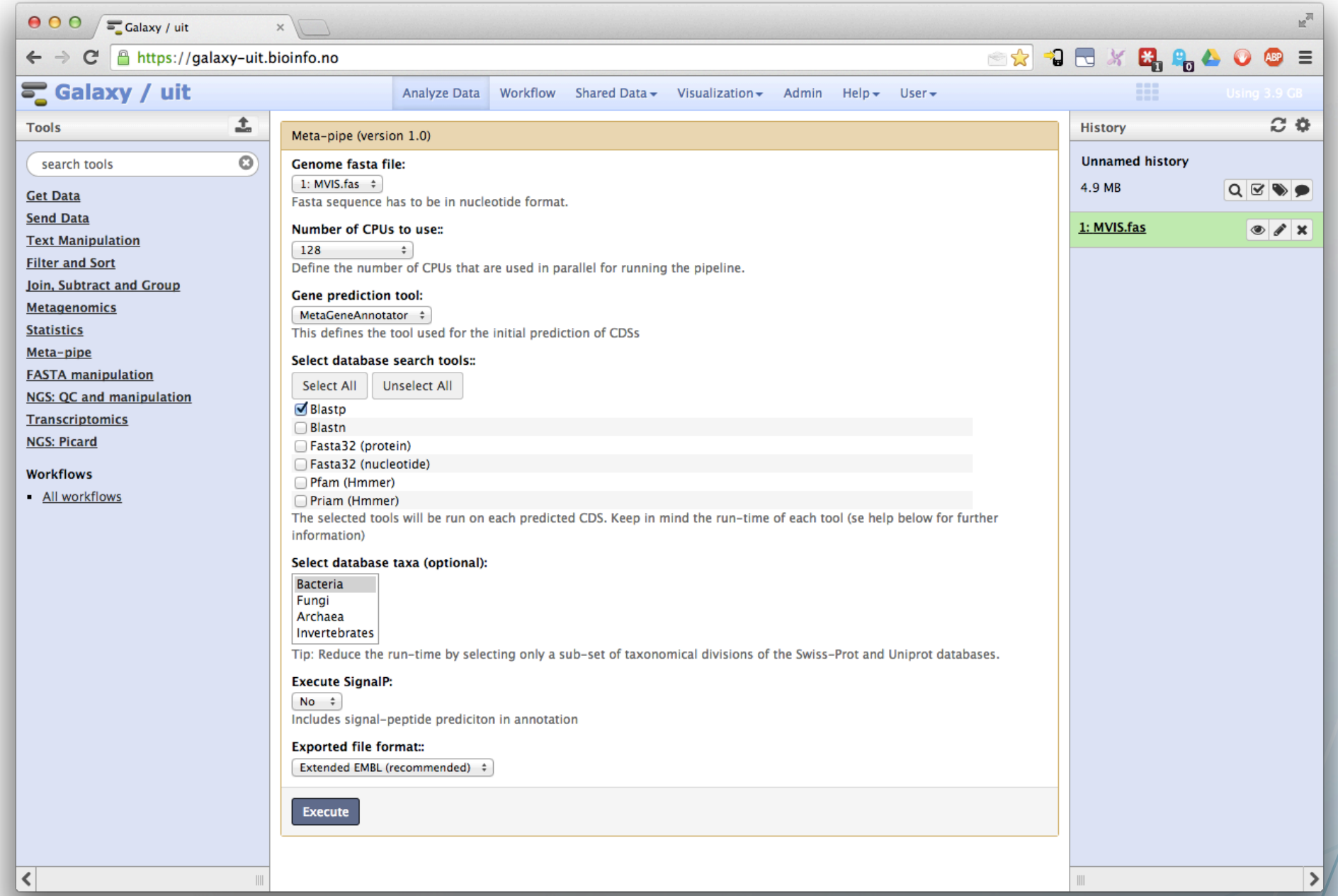
- Increase user base
  - Storage and compute requirements?
  - Where to store data for European users?
  - EBI MGP usage logs can be used to predict requirements
  - Pipelines and infrastructure scalable wrt number of users
  - HPC group at UiT not worried wrt available resources
- Reduce response time
  - What are the requirements and promises to users?
  - Improved algorithms, optimized data structures, dedicated cluster nodes?, Hadoop type of cluster?
- Single sign-in for all users
  - Accounting? Who is paying?
  - Academic vs. commercial users (licences, etc)?
  - Work in progress in NeLS
  - Need to decide and implement policies

Ongoing Work and Challenges

- Improved fault tolerance for 24/7 service
- Stallo cloud
  - OpenStack
  - Well suited for interactive jobs
- Large meta-database management
- Avoid Stallo bottlenecks
  - Scheduler
  - NAS/ Centralized storage
  - CPU (for some tools)
- Non-Galaxy web-interface
  - Remove many potential failures
  - Easier to predict resource usage
- Harmonization with EBI MGP

Use Case Deliverables

- Specific marine databases made publicly available
- Report on comprehensive metagenomic data standards environment
- Report describing a set of tools, pipelines and search engine for interrogation of marine metagenomic


Galaxy / uit
https://galaxy-uit.bioinfo.no
Galaxy / uit
Analyze Data
Workflow
Shared Data
Visualization
Admin
Help
User
Using 3.9 GB
Tools
search tools
Get Data
Send Data
Text Manipulation
Filter and Sort
Join, Subtract and Group
Metagenomics
Statistics
Meta-pipe
FASTA manipulation
NGS: QC and manipulation
Transcriptomics
NGS: Picard
Workflows
All workflows
Meta-pipe (version 1.0)
Genome fasta file:
1: MVIS.fas
Fasta sequence has to be in nucleotide format.
Number of CPUs to use::
128
Define the number of CPUs that are used in parallel for running the pipeline.
Gene prediction tool:
MetaGeneAnnotator
This defines the tool used for the initial prediction of CDSs
Select database search tools::
Select All
Unselect All
Blastp
Blastn
Fasta32 (protein)
Fasta32 (nucleotide)
Pfam (Hmmer)
Priam (Hmmer)
The selected tools will be run on each predicted CDS. Keep in mind the run-time of each tool (se help below for further information)
Select database taxa (optional):
Bacteria
Fungi
Archaea
Invertebrates
Tip: Reduce the run-time by selecting only a sub-set of taxonomical divisions of the Swiss-Prot and Uniprot databases.
Execute SignalP:
No
Includes signal-peptide prediciton in annotation
Exported file format::
Extended EMBL (recommended)
Execute
History
Unnamed history
4.9 MB
1: MVIS.fas

Oppdatert figur (EBI vs. M-P)