ifb
INSTITUT FRANÇAIS DE BIOINFORMATIQUE

METABOHUB

4 Wm

Workflow4metabolomics

cnrs

SCIENCES SORBONNE UNIVERSITÉ

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la science pour la vie, l'humain, la terre

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W4M

DUBii - 2021

Mélanie Pétéra

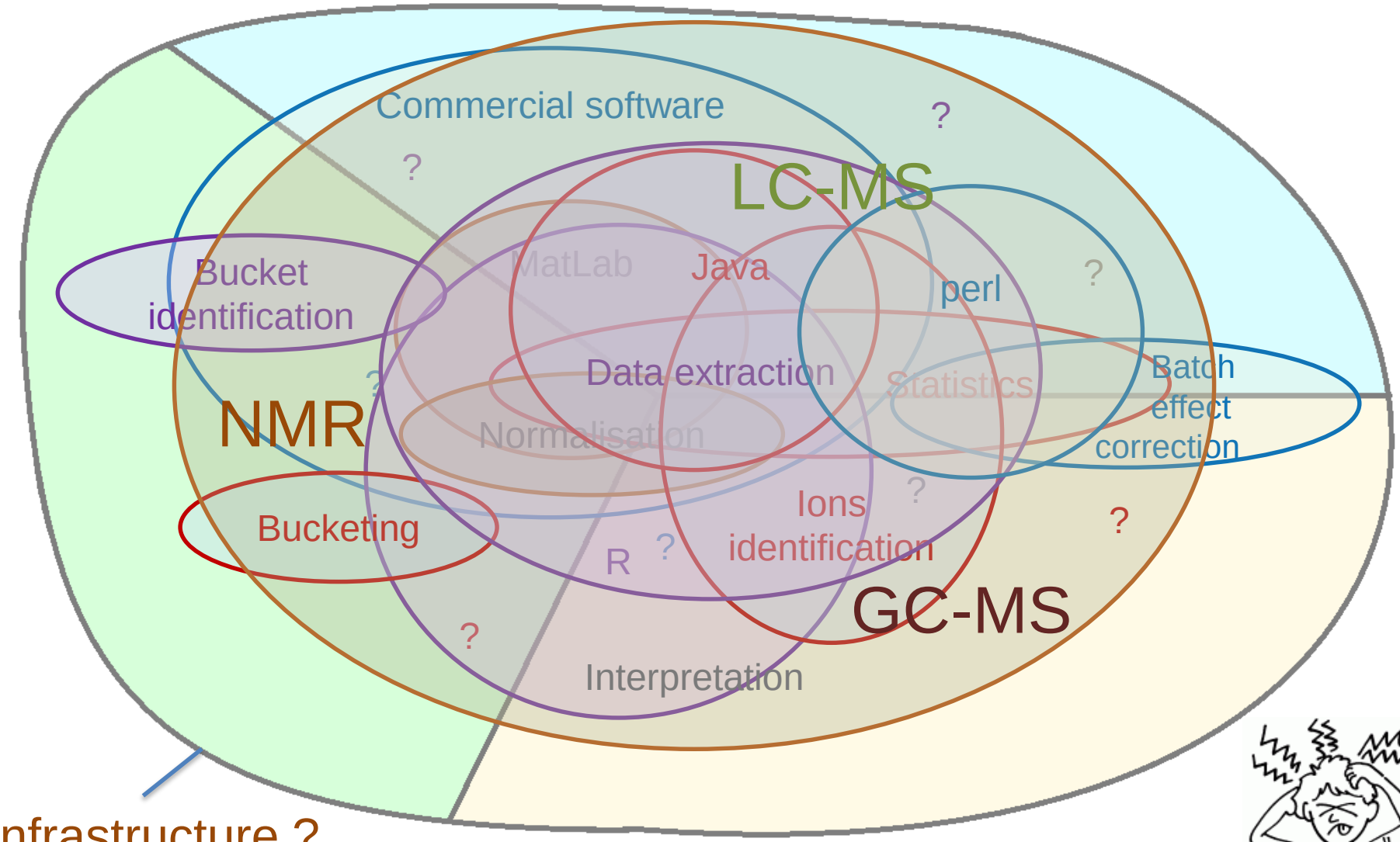
22/03/2021

v 1.0.0

Workflow4Metabolomics – W4M

POURQUOI ?

Une multitude d'outils



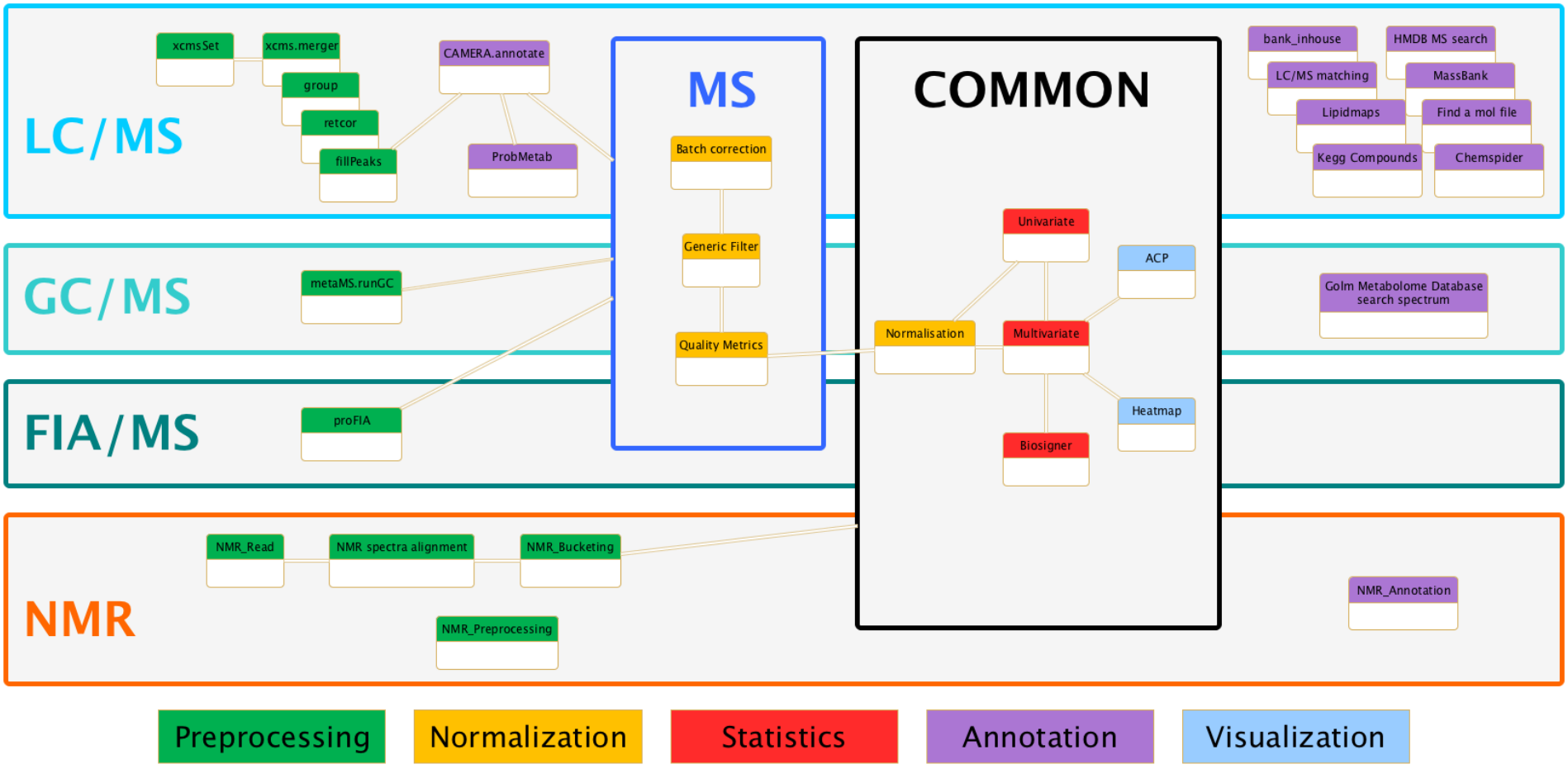
Infrastructure ?

COMMENT ?

W4M – un travail collaboratif

- Un partenariat entre plusieurs structures dont MetaboHub et l'IFB (infrastructures d'avenir)
- Développement d'outils autour de la métabolomique : RMN, MS
- Mise à disposition de ces outils pour pouvoir traiter les données « de A à Z »

Des outils mis en commun pour couvrir l'essentiel



Le choix de Galaxy

https://galaxyproject.org/

Gestionnaire de workflow

Galaxy

Data Intensive *analysis* for everyone

- Versatile and reproducible workflows
- **Web** platform
- **Open source** under Academic Free License
- Developed at Penn State, Johns Hopkins, OHSU and Cleveland Clinic with substantial outside contributions

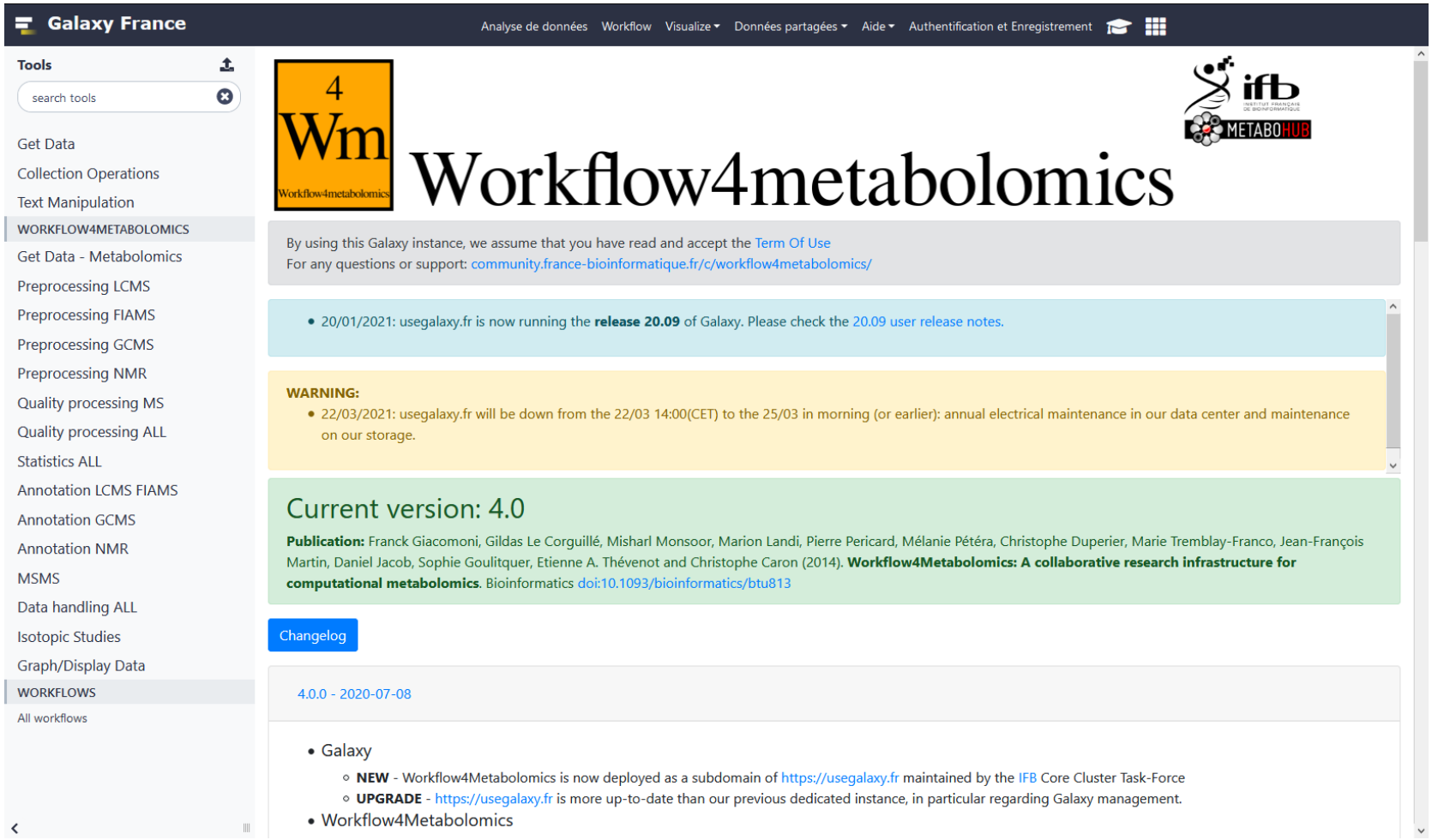
https://training.galaxyproject.org/training-material/topics/introduction/slides/introduction.html#3

Le choix de Galaxy

Un équilibre entre besoins des utilisateurs et des pourvoyeurs d'outils

User advantages	Developer advantages
√ GUI	√ Easy integration of tools
√ Ergonomics	√ Multi-language
√ Modularity	√ Collaborative development
√ Reproducibility	√ Open-source
√ Data & workflow sharing	√ Possibility of link with external ressources
√ Possibility of new tools' integration	

Un sous-domaine dédié sur l'instance nationale usegalaxy.fr



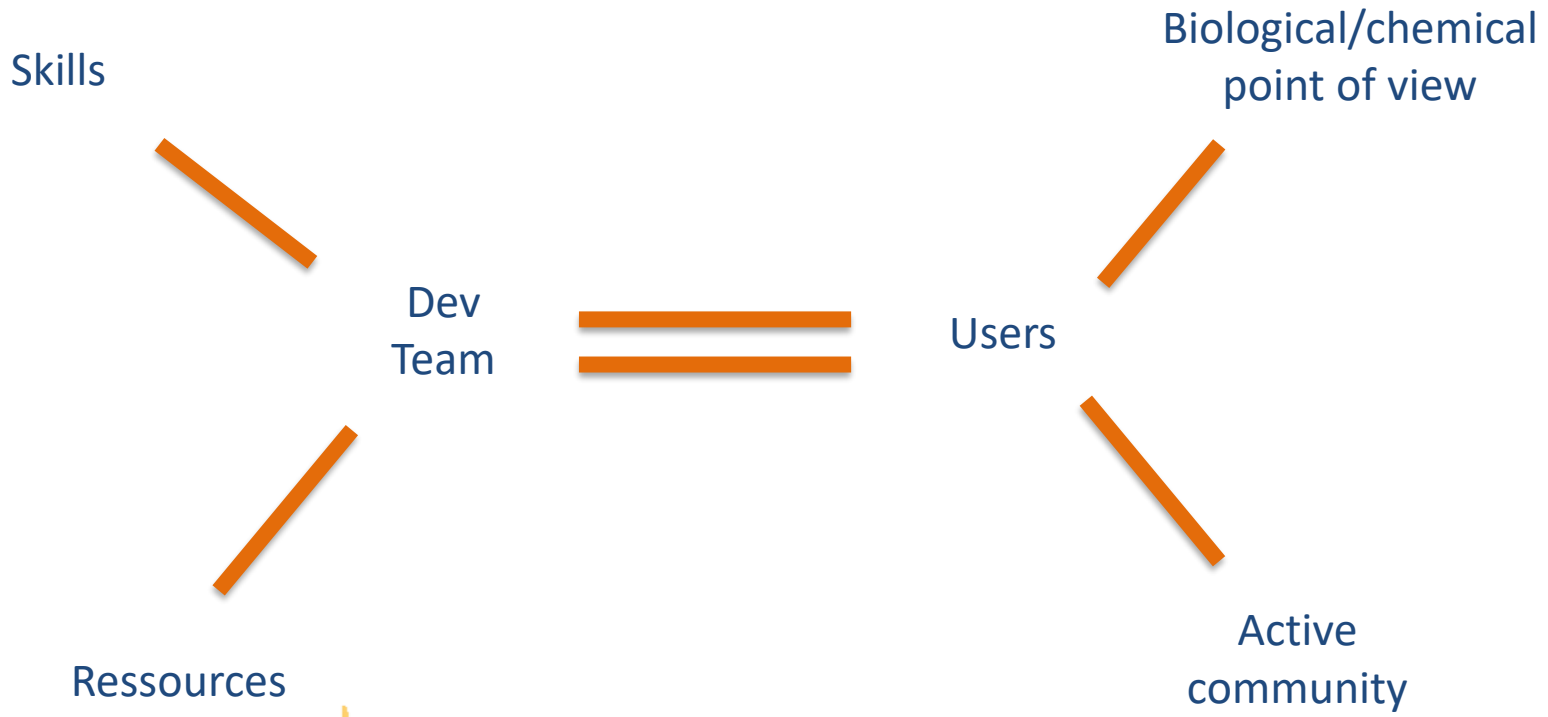
https://workflow4metabolomics.usegalaxy.fr/

UNE COMBINAISON GAGNANTE !

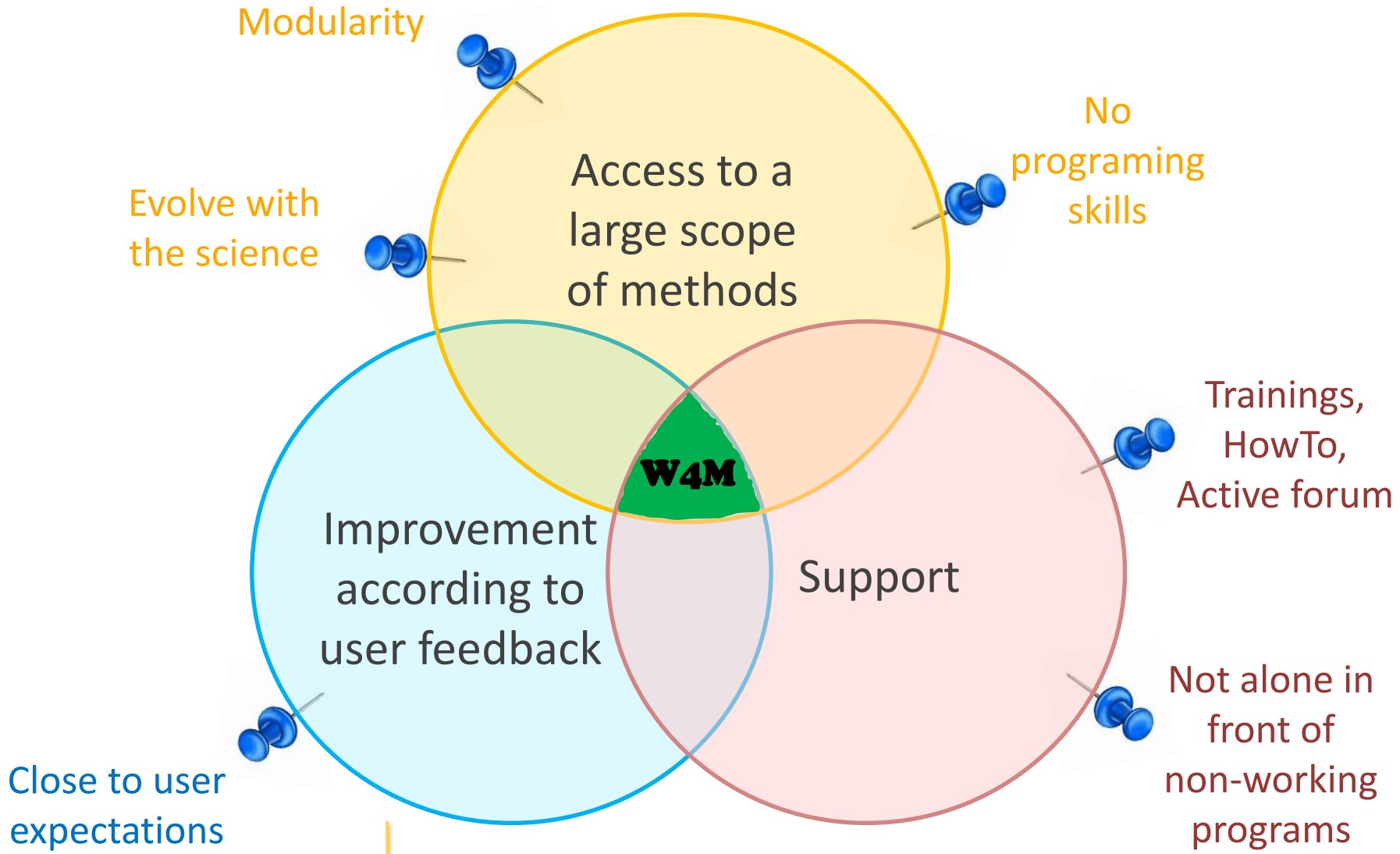
La chimie de W4M

Our equation

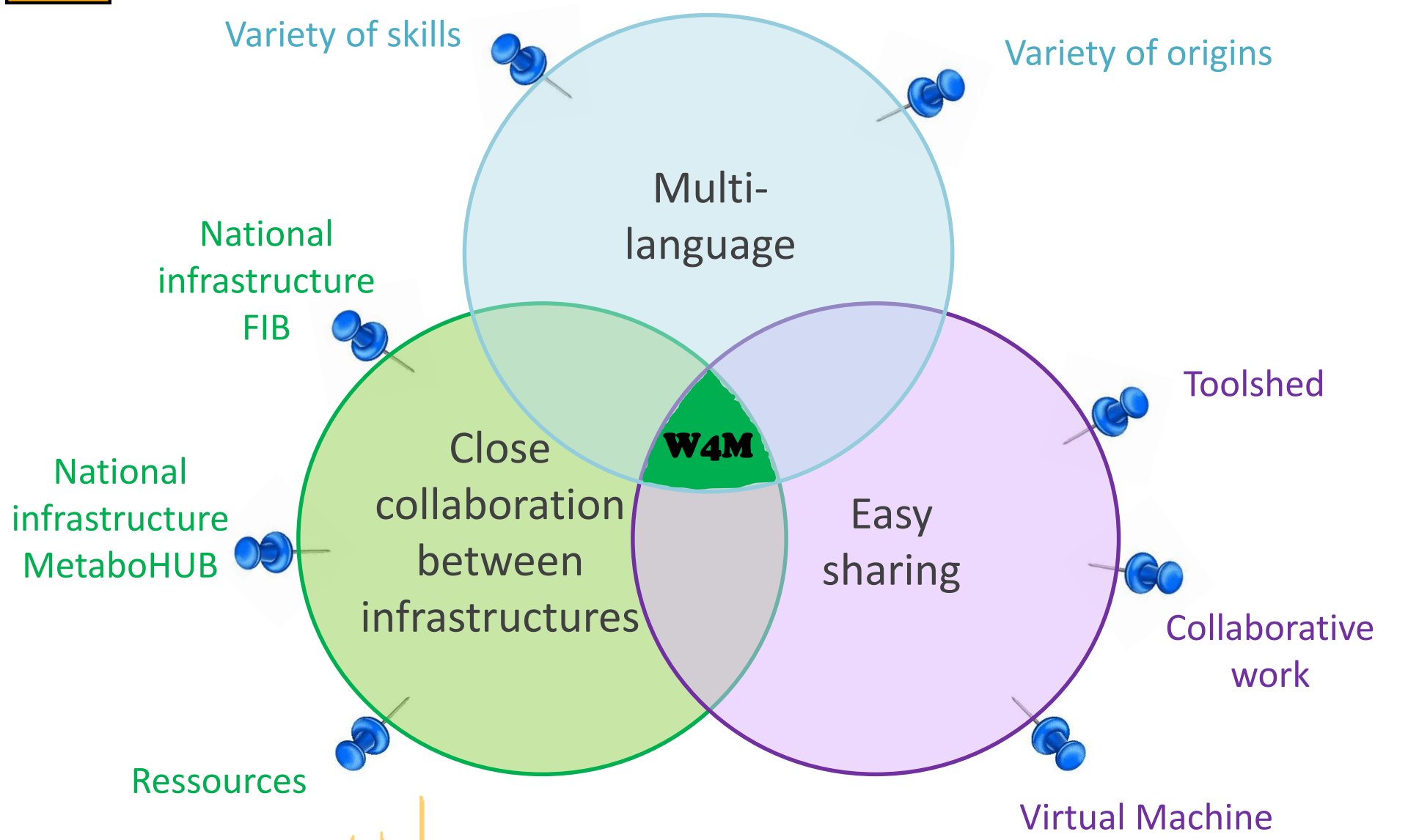
Easy access to existing tools + Development of new tools + Easy handling for users → W4M



Efficace pour les utilisateurs



Efficace pour les développeurs



Pour aller plus loin

https://workflow4metabolomics.org/

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Applications Note

Gene expression

Workflow4Metabolomics: a collaborative research infrastructure for computational metabolomics

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Abstract

Summary: The complex, rapidly evolving field of computational metabolomics calls for collaborative infrastructures where the large volume of new algorithms for data pre-processing, statistical analysis and annotation can be readily integrated whatever the language, evaluated on reference datasets and chained to build ad hoc workflows for users. We have developed Workflow4Metabolomics (W4M), the first fully open-source and collaborative online platform for computational metabolomics. W4M is a virtual research environment built upon the Galaxy web-based platform technology. It enables ergonomic integration, exchange and running of individual modules and workflows. Alternatively, the whole W4M framework and computational tools can be downloaded as a virtual machine for local installation.

Availability and implementation: http://workflow4metabolomics.org homepage enables users to open a private account and access the infrastructure.

W4M is developed and maintained by the French Bioinformatics Institute (IFB) and the French Metabolomics and Fluxomics Infrastructure (MetaboHUB).

Contact: contact@workflow4metabolomics.org

1 Introduction

Metabolomics, the high throughput analysis of small molecules in biological samples, heavily depends on data pre-processing, statistical analysis and chemical and biological annotation, which are complex, transdisciplinary processes involving both computation volume of proposed algorithms written in various languages, making their evaluation by the bioinformatics community (including reviewers) and their chaining within ad hoc workflows by experimenters difficult (Smith *et al.*, 2013).

A few user-oriented online platforms for metabolomics data pre-

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Create, run, share, publish, and reference your LC–MS, FIA–MS, GC–MS, and NMR data analysis workflows with the Workflow4Metabolomics 3.0 Galaxy online infrastructure for metabolomics

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ABSTRACT

Metabolomics is a key approach in modern functional genomics and systems biology. Due to the complexity of metabolomics data, the variety of experimental designs, and the multiplicity of bioinformatics tools, providing experimenters with a simple and efficient resource to conduct comprehensive and rigorous analysis of their data is of utmost importance. In 2014, we launched the Workflow4Metabolomics (W4M; http://workflow4metabolomics.org) online infrastructure for metabolomics built on the Galaxy environment, which offers user-friendly features to build and run data analysis workflows including preprocessing, statistical analysis, and annotation steps. Here we present the new W4M 3.0 release, which contains twice as many tools as the first version, and provides two features which are, to our knowledge, unique among online resources. First, data from the four major metabolomics technologies (i.e., LC–MS, FIA–MS, GC–MS, and NMR) can be analyzed on a single platform. By using three studies in human physiology, alga evolution, and animal toxicology, we demonstrate how the 40 available tools can be easily combined to address biological issues. Second, the full analysis (including the workflow, the parameter values, the input data and output results) can be referenced with a permanent digital object identifier (DOI). Publication of data analyses is of major importance for robust and reproducible science. Furthermore, the publicly shared workflows are of high-value for e-learning and training. The Workflow4Metabolomics 3.0 e-infrastructure thus not only offers a unique online environment for analysis of data from the main metabolomics technologies, but it is also the first reference repository for metabolomics workflows.