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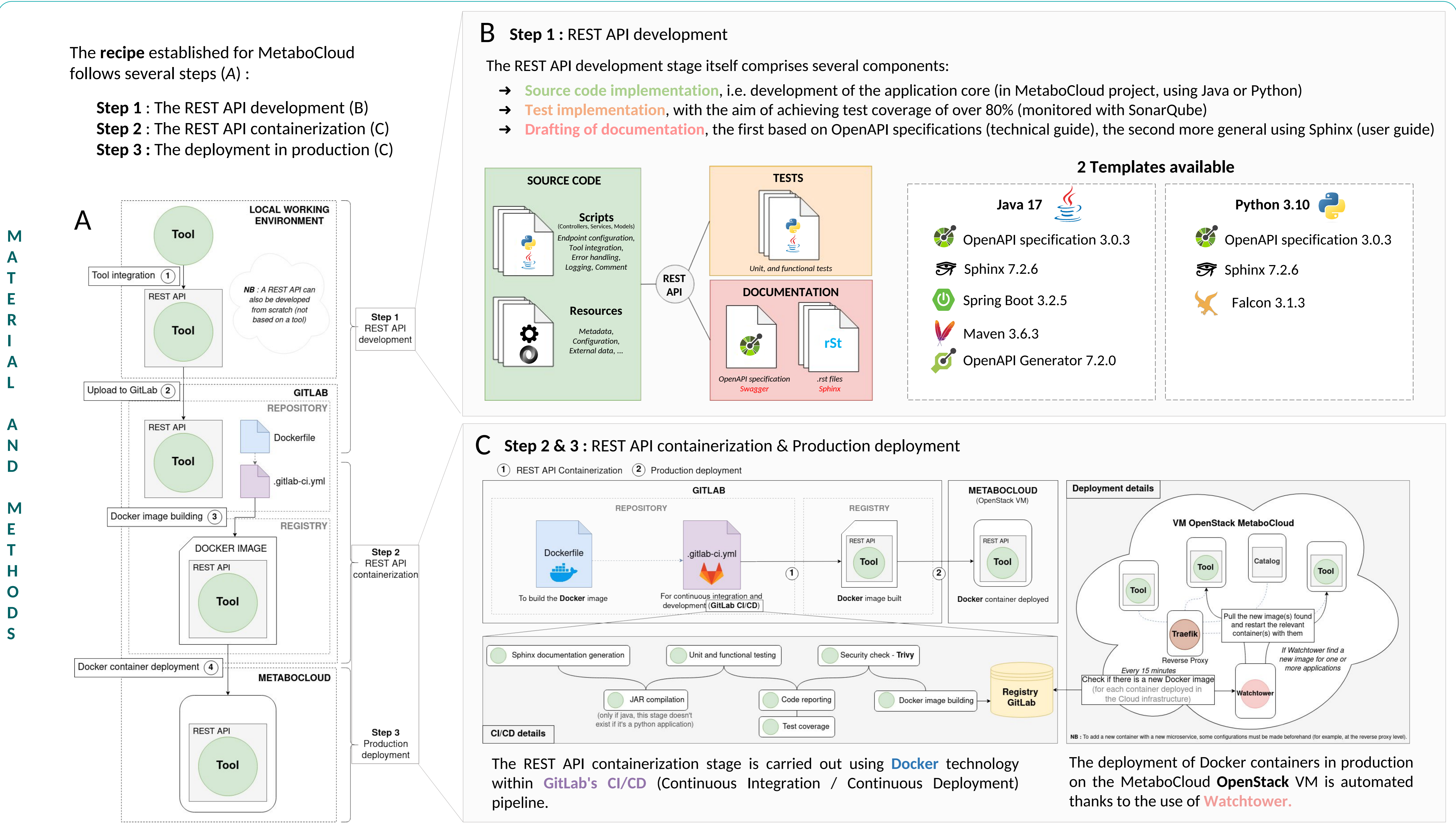
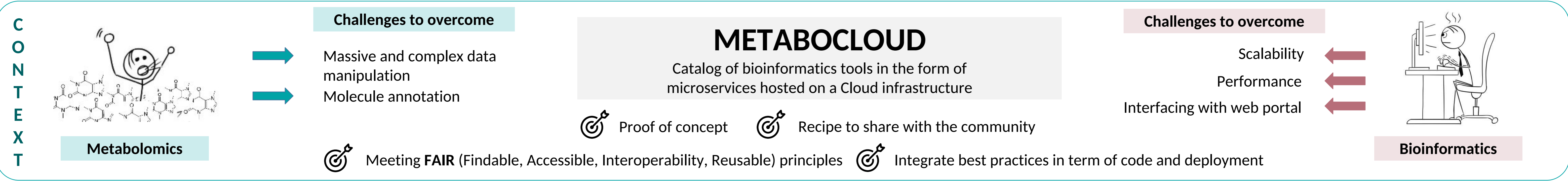
MetaboCloud : A catalog of microservices hosted on a Cloud infrastructure and addressing issues linked to FAIR principles and open science.

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Three microservices are currently available via the web portal MetaboCloud.

- Goslin^[1] ("Grammar On Succinct Lipid Nomenclature") microservice developed in python 3.10 from **pygoslin 2.1.0**
- CDK^[2] ("Chemistry Development Kit") microservice developed in java 17 from **CDK 2.9**
- InChI^[3] microservice developed in java 17 from the binary program **InChI 1.06**

Goslin

Translate lipid names into standardized names

GET /about **GET /grammars** **GET /validate**

Input : ∅ ∅ Lipid name

Output : Metadata Grammars list Lipid name standardization

InChI

Produce InChI/InChI Key of chemical compounds

GET /about **POST /generation**

Input : ∅ InChI/MOL/SDF

Output : Metadata Generate the compound InChI/InChI Key

CDK

Compute chemical properties, depict or convert a molecule

GET /about **POST /properties** **POST /depiction/{format}** **POST /conversion/{format}**

Input : ∅ InChI/MOL/SDF InChI/MOL/SDF InChI/MOL/SDF

Output : Metadata Chemical properties Visual representation of the compound Convert to another format

Catalog

<https://metabocloud.mesocentre.uca.fr>

Application building the MetaboCloud web portal, which list all available microservices with their metadata and documentation.

Web Components
Ready-to-use client to insert into a HTML page

Batch Mode
Single or combined use of microservices via scripts

Application
Construction of an application based on microservices architecture

The MetaboCloud microservices infrastructure is based on :

- Bioinformatic tools
- From scratch API development if tools are not available
- Quality testing and documentation
- An advanced CI/CD work environment managing the construction of a docker image
- Taken all together in an OpenStack cloud technology environment

Findable → Web portal associated with metadata (FAIRChecker evaluation)

Accessible → Metadata and documentation for each microservice

Interoperable → Can be queried from any programming language, work environment, ...

Reusable → Version control through containerization

WHAT'S NEXT?

- Development of new microservices
- Maintaining current microservices
- Hackathons directed to developers/users
- Current development : a microservice to retrieve PNG and MOL stored in a S3 storage

References: [1] Kopczyński D, et al. 2022 *Anal Chem*. Apr 26;94(16):6097-101. [2] Willighagen EL, et al. 2017 *J Cheminformatics*. Dec;9(1):33. [3] Heller SR, et al. 2015 *J Cheminformatics*. May 30;7:23. [4] Emami Khoonsari P, et al. 2019 *Bioinformatics*. Oct 1;35(19):3752-3760.

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