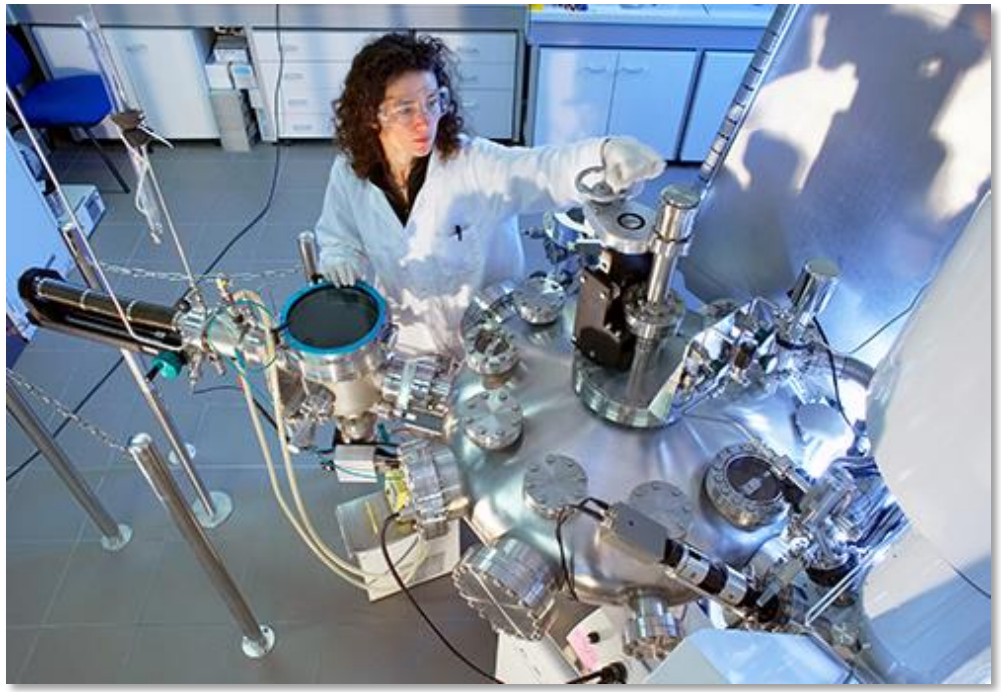


IFPEN

How open-source projects have been made possible by CC ASM

va

ifp Energies nouvelles

WHAT DOES IFPEN WANTS TO ACHIEVE WITH ASM?

Internal efficiency

- Larger data sets for data engineers
- Reusability of tools across the company

Be a key player in the energetical, evironmental and digital transition

- Facilitating the use of experimental data (open data)
- Facilitating the use of our tooling (open source)

USE CASE

Lab A developped a web app to visualize and interpret IR data.
Their software saves data as .spc files

Lab B reaches out to IT, asking for a web app to visualize and interpret IR data.
Their software saves data as .jdx files

⇒Start corporate project to push IR data to the data-lake, and tweak the web-app to read ASM compliant JSON files.

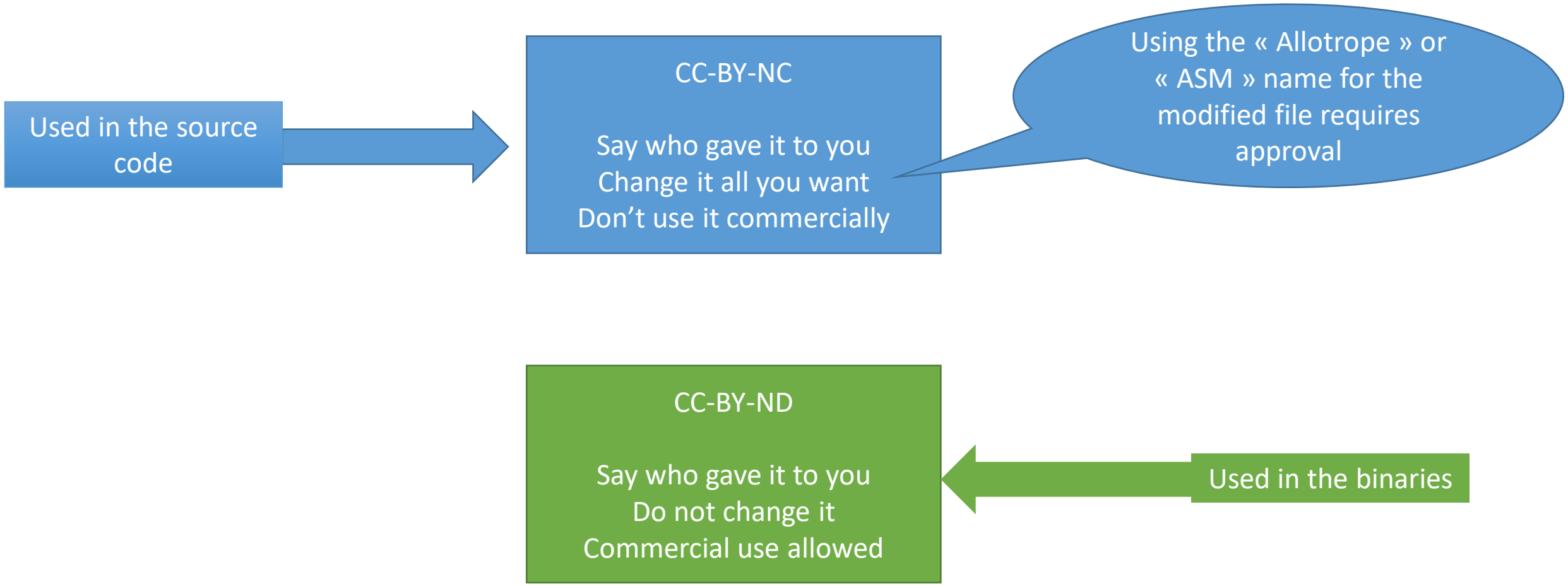
⇒Switch from file-by-file parsing in the browser to industrial ingestion of data in the data-lake (Java program, running in a container managed by a Kubernetes infrastructure)

OPEN SOURCE

- The parsing algorithm used is translated from existing open-source implementations (R for NMR, Python for Chemstation GC or SPC IR, Java for JDX IR), licenced under GPL or similar licence.
  - The converter libraries are derivative code, and are subject to the GPL licence
  - The converter libraries use the ASM schema files (to generate Java DTOs and to validate generated files). The library cannot compile without the ASM schema files.

With closed source ASM
the path of open science stops here

2023: ADM RELEASED UNDER CREATIVE COMMONS LICENCE



OPEN SOURCE ALLOTROPE CONVERTERS

IFPEN released two open-source projects:

GC2ASM (https://github.com/ifpen/GC2ASM) – a converter for GC files

IR2ASM (https://github.com/ifpen/IR2ASM) – a converter for IR files

All projects are available on Maven Central, in the fr.ifpen.allotropeconverters namespace

With many more on the roadmap:

A converter for NMR files

A web-service for serving Chromeleon Entreprise data

DEMONSTRATION

How to convert a ChemStation .D file into an ASM compliant JSON file.

https://github.com/ifpen/SpringConnect2023Demo

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