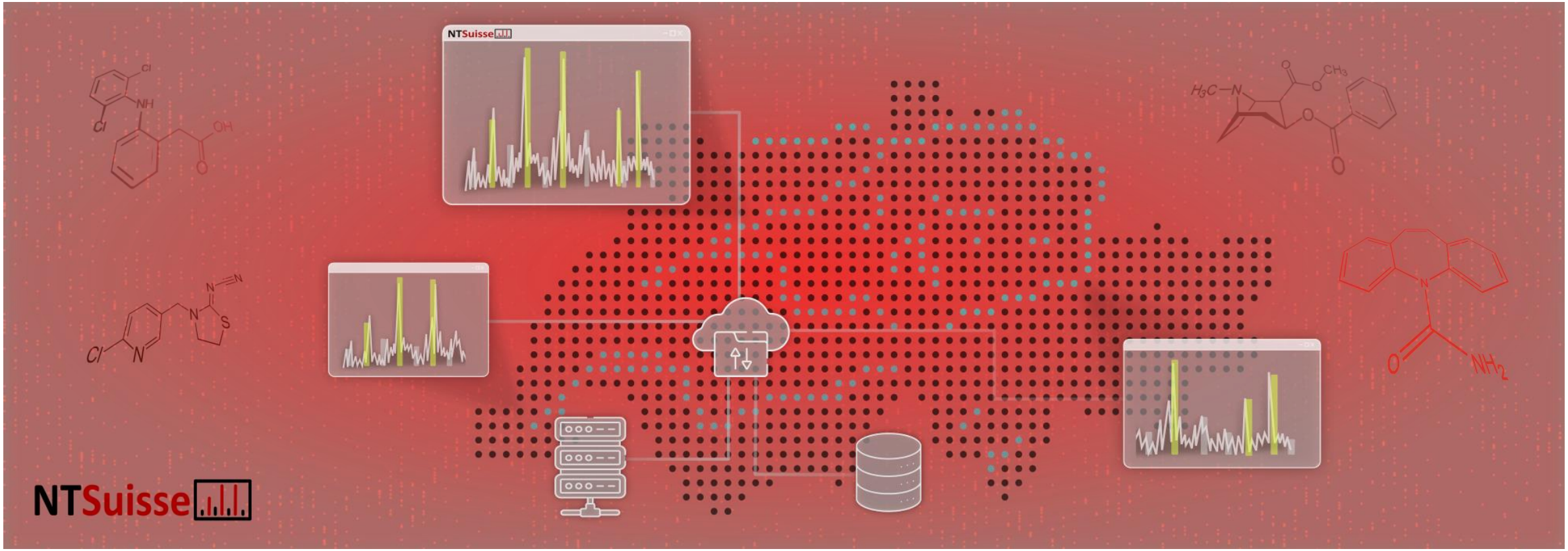
NTSuisse: A Web Platform for Centralized Automatic Processing and Evaluation of Swiss LC-HRMS Surface Water Data



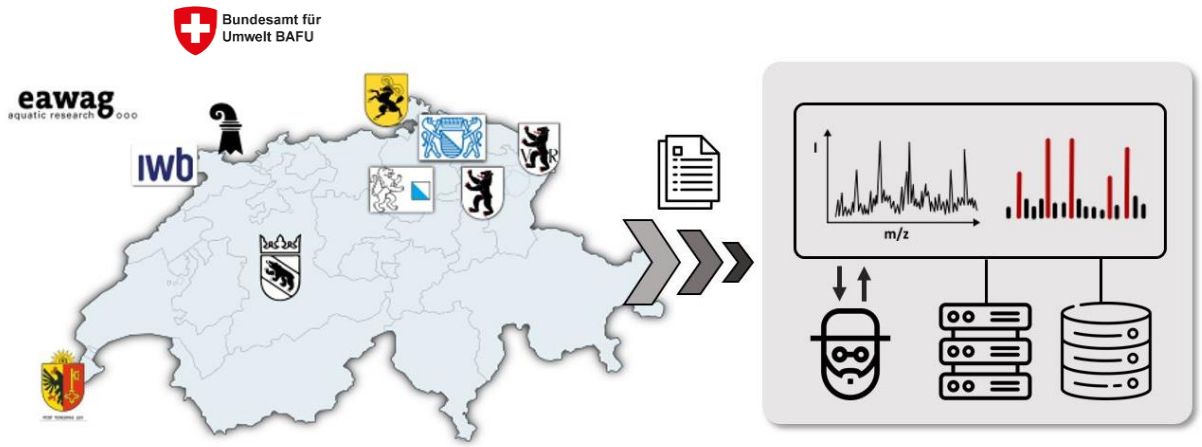
Kai Kammer, Johannes Boog, Fernando Calvo, Sebastian Salzmann, Michele Stravs, Heinz Singer

Eawag, Department Environmental Chemistry

04.09.2025

Project Goals & Overview

- Provide a more comprehensive understanding of chemical pollution of Swiss surface waters
- Compare & exchange data between cantons
- Web platform for uploading, processing, evaluation of Swiss LC-HRMS water data
- 9 Partners
  - Cantonal water protection labs
  - Cantonal water suppliers
  - BAFU
  - Eawag



The Web Platform

- *Simple* web platform of Swiss LC-HRMS surface water data
- Uploading and storage
- Centralized automatic processing
- Target screening
- Evaluation and visualization capabilities
- Data comparison and exchange
- Retrospective screening of new targets

NTSuisse

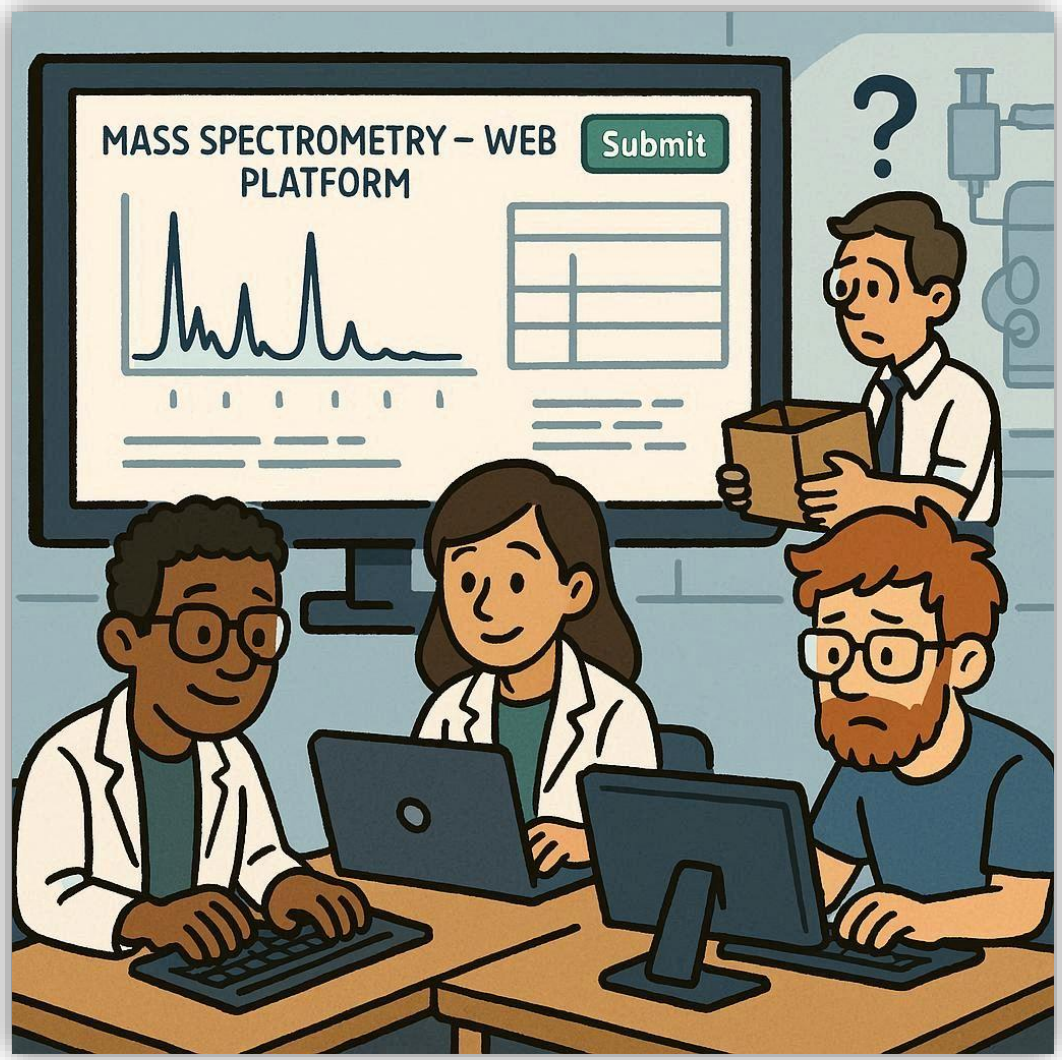
The Timeline

- 2022/10: Planning Start
- 2023/05: Development Start
- 2024/11: I joined
- 2025/12: Delivery of Production Platform
- 2026-2027: Ongoing Support + Feature Development

NTSuisse

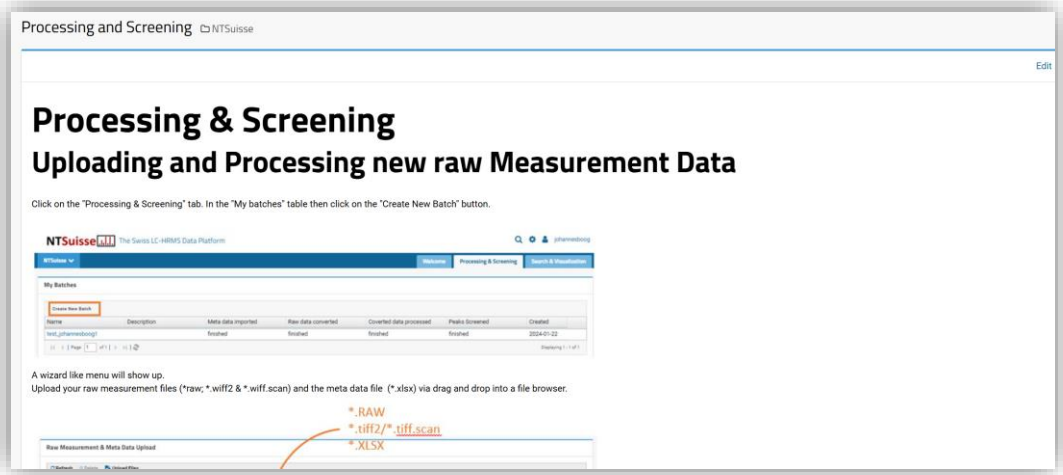
The Dev Team

- 20% Software Engineer: overall project + managing
- 80% Frontend Engineer: frontend + db
- 100% Software Engineer: backend + managing
- Collaboration via gitlab: follow conventional commits, use of merge requests & CI pipelines
- Two former engineers: turnover means documentation is very important

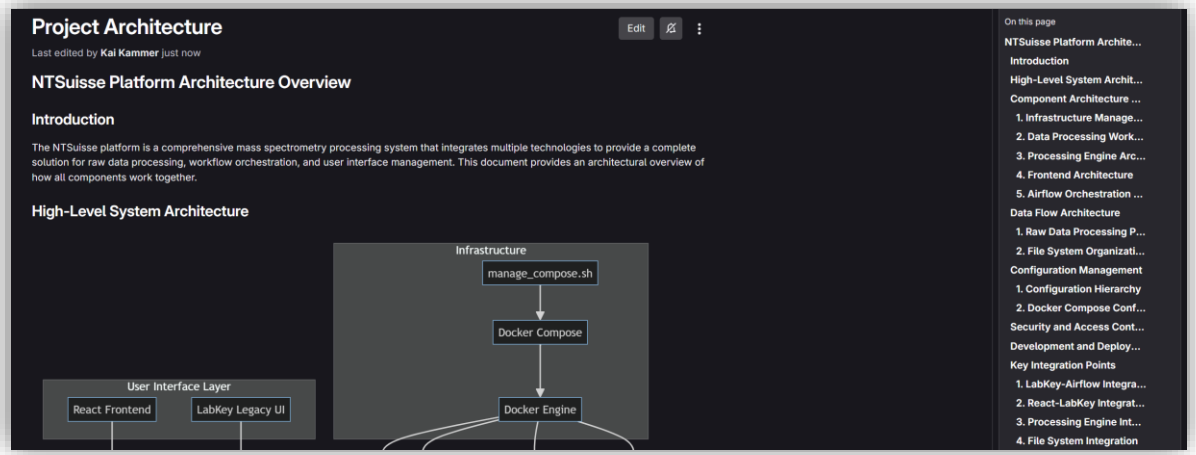


Documentation

- User Wiki & UI Tooltips



- Developer Wiki



- Code Documentation

Platform Architecture – Technology

NTSuisse

Frontend

LabKey®

React JS

plotly

Apache Airflow

Backend

mzmine

proteowizard

PostgreSQL

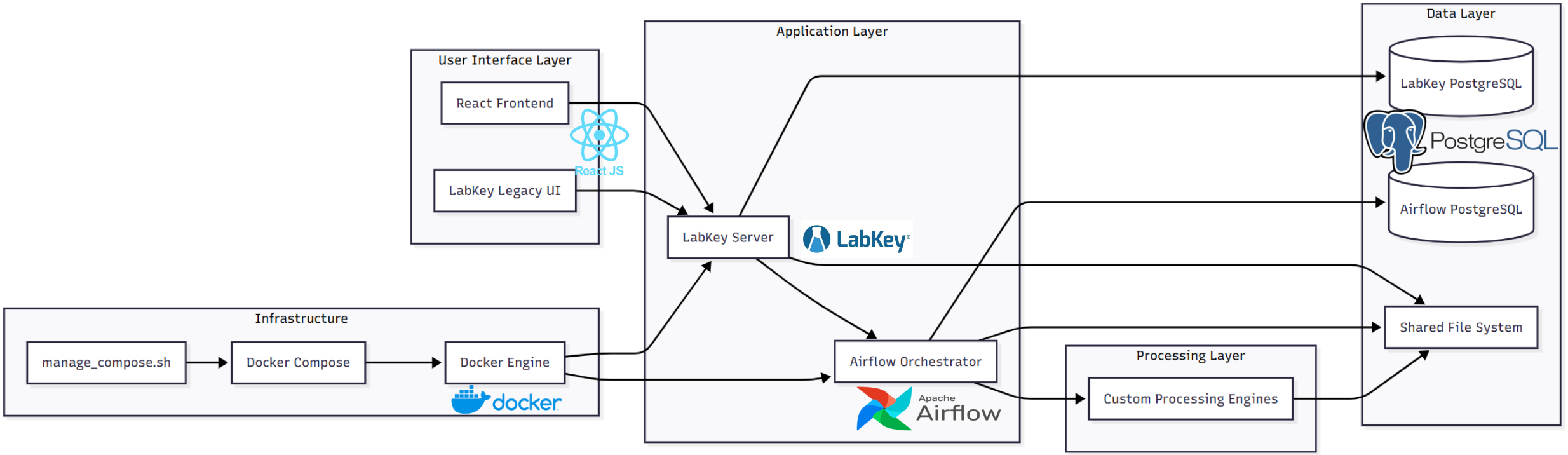
NTSuisse

Live Demo

Finger’s crossed it is actually working…

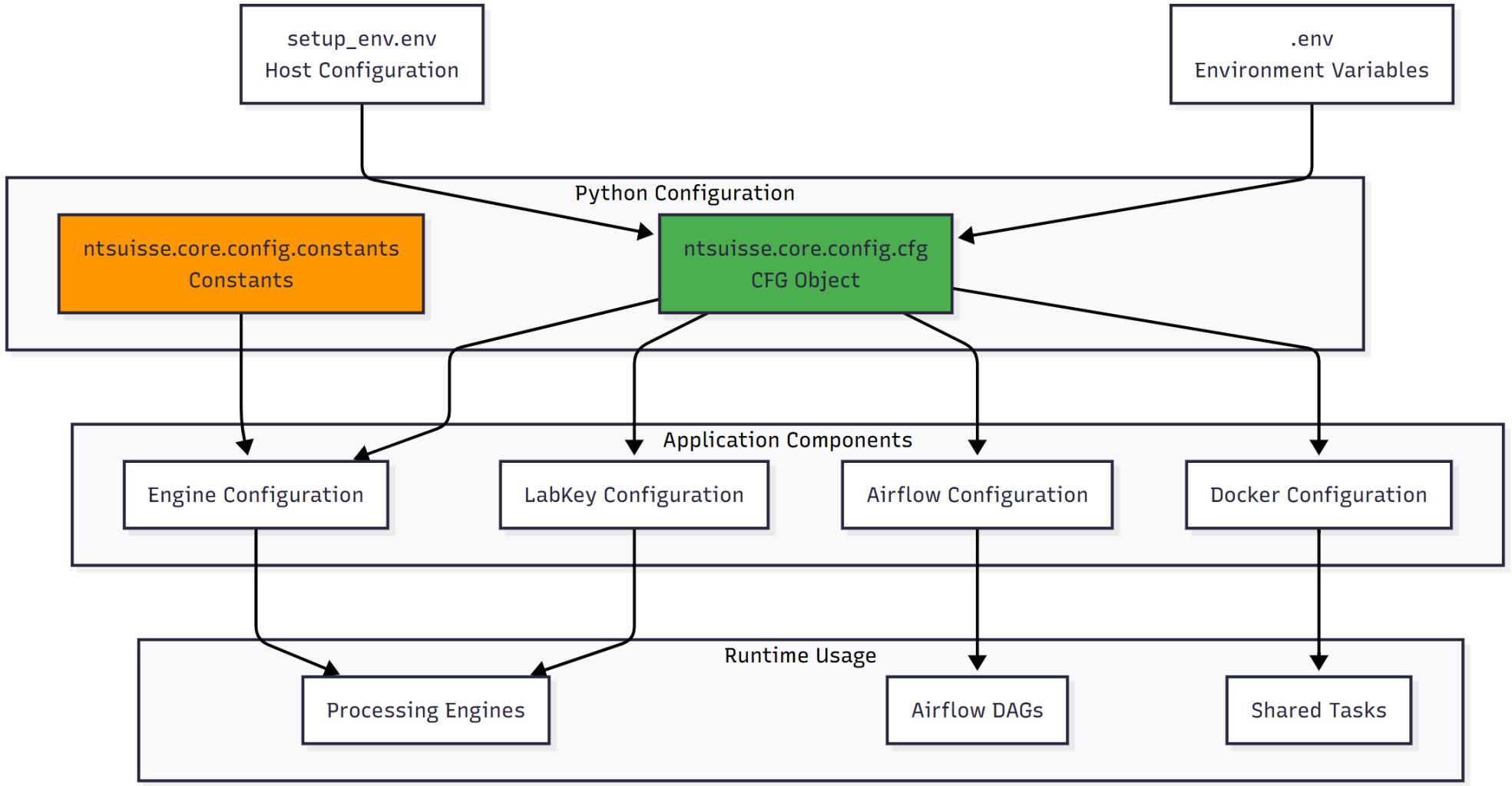
Platform Architecture – Overview

NTSuisse



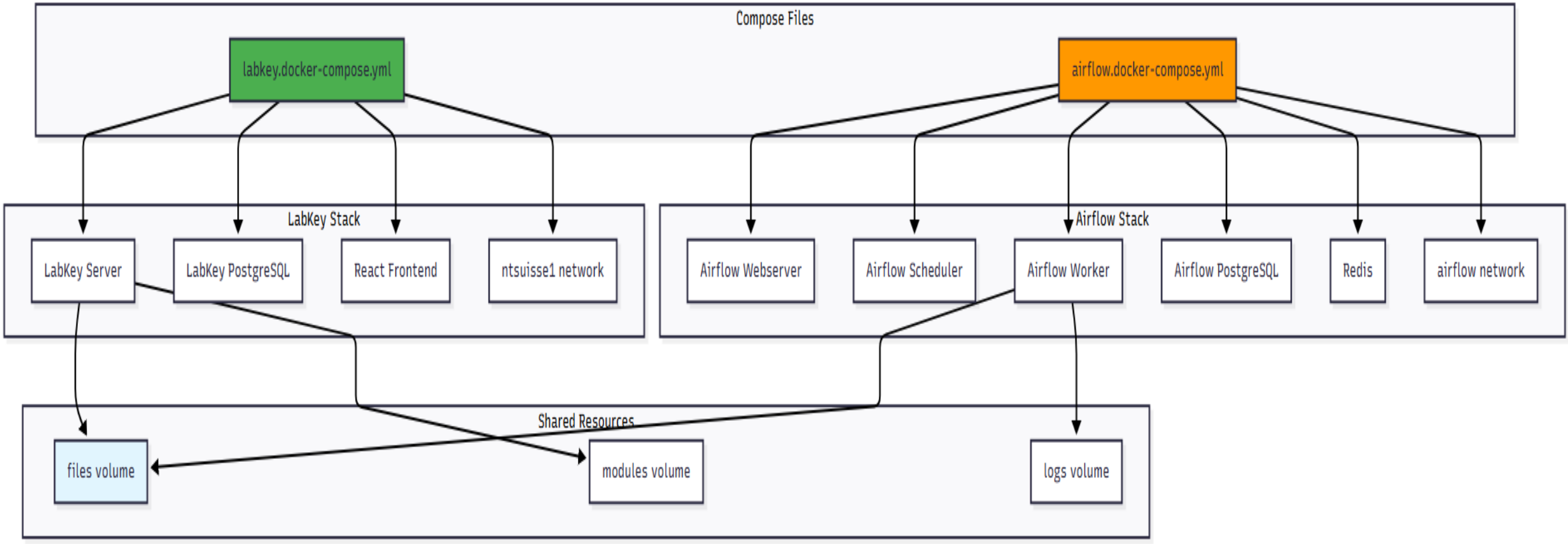
Sore Point – Configuration

NTSuisse



Sore Point – Configuration (docker compose)

NTSuisse



NTSuisse

Main Takeaways

- **Test your code**
  - Or find out late what your last edit did
- **Take your time selecting the tech stack**
  - Otherwise you will spend time removing it later on
- **Comment your code and write documentation**
  - AI tools are useful helpers for that