Development of a flexible, multi-stage data pipeline

... for enhanced automation, quality control and observability

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Current Status ... a patchwork of processes and workflows

- Heterogenuous data processing landscape
- No centralized control/ interface
- No/ limited data processing version control
- No/ limited data QA/ QC
- No centralized data catalog



Objectives ... there has to be a better way

Consolidate

Centralise services, jobs and scripts into a manageable system

Automate

Create data transformation pipelines that take care of data ingestion, auto-validation and transformation (data repositories)

Increase Consistency

A global scheduling ensures that processes run at defined times/ intervals or conditions

Add Scalability

The system should scale from few jobs to actual model processing (i.e. data generation for dashboards etc.)

Add Observability

System status, failure and progress should be easily observable, data owners be notified if things break or are out-of-norm



Proposed solution ... develop an flexible and scalabe dataflow framework



Open-source

Centralized workflows with Prefect

Data publication via STA and THREDDs

Observability via Prefect UI, Grafana, APIs

- Workflows as code (CI/CD pipelines after change)
- Data Quality Checks with GreatExpectations and SaQC

Workflow Orchestration ... schedule and control via Prefect



Example Workflow TERENO micromet ingest, QA/ QC and publication



Prefect Workflow definition (as code)

```
from prefect import flow, task
from typing import List
import httpx
@task(retries=3)
def get_stars(repo: str):
    url = f"https://api.github.com/repos/{repo}"
    count = httpx.get(url).json()["stargazers_count"]
    print(f"{repo} has {count} stars!")
@flow(name="GitHub Stars")
def github_stars(repos: List[str]):
    for repo in repos:
        get_stars(repo)
# run the flow!
github_stars(["PrefectHQ/Prefect", "PrefectHQ/miter-design"])
```


Task and flow definition as code

Quality Control I Great Expectations - Data Profiling and initial QC

- Initial automated profiling on existing valid data
- Define "expectations"
- Checks preformed at ingest time (8am), alert if missing data and other expectations are not met
- Valid data ingested into FROST staging server [LVL1]

Your data assets: database tables, flat files, dataframes...

High quality data in your data products

Data documentation & data quality reports

Logging & alerting

Basic Profiling on new data batches and promotion to Level 1 status

Quality Control II SaQC - measurement/ project-specific QC

- Manual intervention step at weekly interval
- Domain knowledge required
- Checks performed on time-span of data (data drift detection, outliers etc.)
- After approval data accessible via STA from 2nd FROST server [LVL2]

Data Access Sensor Things API

- Data access via STA API (REST or via code, i.e. stantic)
- Grafana) Dashboards

Data Access THREDDS Data Server

- Aggregated datasets [LVL3] (csv, netCDF, monthly/ annual)
- Automatically expand data catalog
- Intake catalog
- Harvested into searchable Geoserver and/ or Data Portal

Catalog http://thredds.ucar.edu/thredds/catalog.htm
Realtime data from IDD
Forecast Model Data/
Forecast Products and Analyses/
Observation Data/
Radar Data/
Satellite Data/
Other Unidata Data
Unidata case studies/

THREDDS Data Server at Unidata see Info THREDDS Data Server [Version 4.6.14 - 2019-07-23T11:04:31-0600] Documentation

Data access through THREDDS Data Server

Workflow Orchestration ... schedule and control via Prefect

References

- FROST Server: <u>https://fraunhoferiosb.github.io/FROST-Server</u>
- Great Expectations: <u>https://greatexpectations.io</u>
- Intake: <u>https://intake.readthedocs.io</u>
- OGC Sensor Things API: <u>https://www.ogc.org/standards/sensorthings</u>
- Prefect: <u>https://prefect.io</u>
- Stantic: <u>https://cwerner.github.io/stantic</u>
- THREDDS Data Server: <u>https://www.unidata.ucar.edu/software/tds</u>

System for automated Quality Control (SaQC): <u>https://rdm-software.pages.ufz.de/saqc</u>