Nyarlathotep

Automated Data Pipelines for eLabFTW

Phillip Seeber

Tuesday 23rd September, 2025

FRIEDRICH-SCHILLER-UNIVERSITÄT JENA

Motivation

- Automate processing of data with eLabFTW

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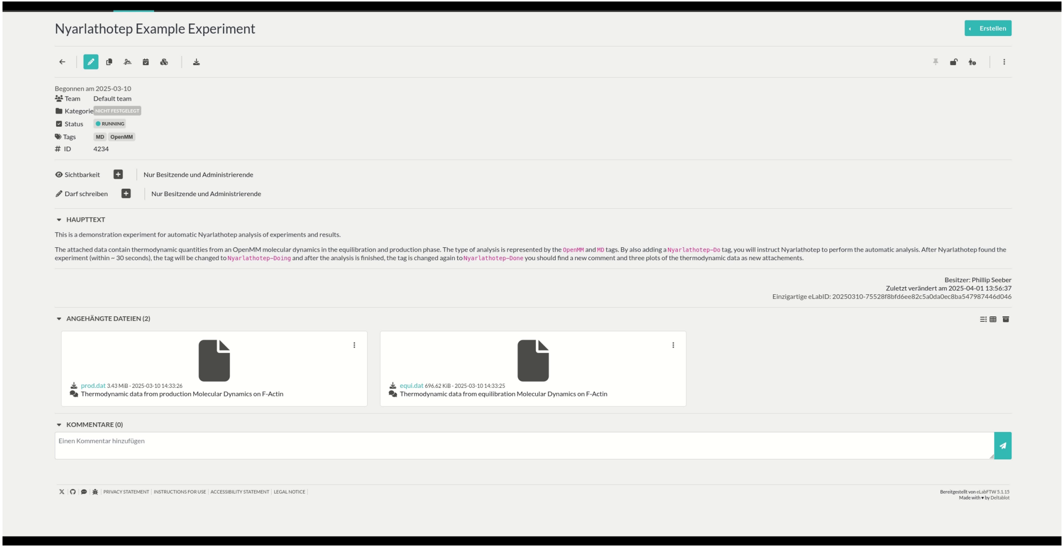
- Enhances traceability and reproducibility of processing
- Possibly eliminates installation of complex software stacks on local machines
- Inspiration: NOMAD Oasis, Chemotion, or GitHub/GitLab CI pipelines



Nyarlathotep Example Experiment

Begonnen am 2025-03-10

Team	Default team
Kategorie	NICHT FESTGELEGT
Status	RUNNING
Tags	MD OpenMM
# ID	4234

Sichtbarkeit: Nur Besitzende und Administrierende

Darf schreiben: Nur Besitzende und Administrierende

HAUPTTEXT

This is a demonstration experiment for automatic Nyarlathotep analysis of experiments and results.

The attached data contain thermodynamic quantities from an OpenMM molecular dynamics in the equilibration and production phase. The type of analysis is represented by the `OpenMM` and `MD` tags. By also adding a `Nyarlathotep-Do` tag, you will instruct Nyarlathotep to perform the automatic analysis. After Nyarlathotep found the experiment (within ~ 30 seconds), the tag will be changed to `Nyarlathotep-Doing` and after the analysis is finished, the tag is changed again to `Nyarlathotep-Done` you should find a new comment and three plots of the thermodynamic data as new attachements.

Besitzer: Phillip Seeber
Zuletzt verändert am 2025-04-01 13:56:37
Einzigartige eLabID: 20250310-75528f8bfd6ee82c5a0da0ec8ba547987446d046

ANGEHÄNGTE DATEIEN (2)

prod.dat 3.43 MiB - 2025-03-10 14:33:26
Thermodynamic data from production Molecular Dynamics on F-Actin

equi.dat 696.62 KiB - 2025-03-10 14:33:25
Thermodynamic data from equilibration Molecular Dynamics on F-Actin

KOMMENTARE (0)

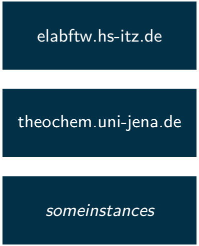
Einen Kommentar hinzufügen

PRIVACY STATEMENT | INSTRUCTIONS FOR USE | ACCESSIBILITY STATEMENT | LEGAL NOTICE
Bereitgestellt von eLabFTW 5.1.15
Made with ♥ by Deltablot

Components

elabftw.hs-itz.de

Components


elabftw.hs-itz.de

theochem.uni-jena.de

someinstances

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Nyarlathotep

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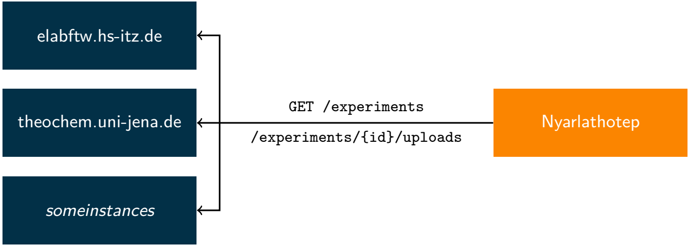
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someinstances
GET /experiments
/experiments/{id}/uploads
Nyarlathotep

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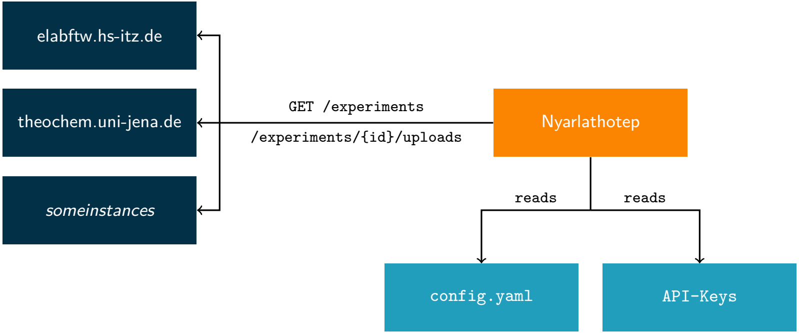
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Nyarlathotep
reads
reads
config.yaml
API-Keys

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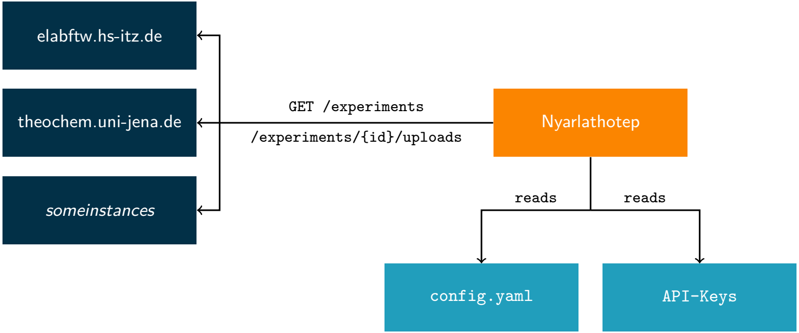
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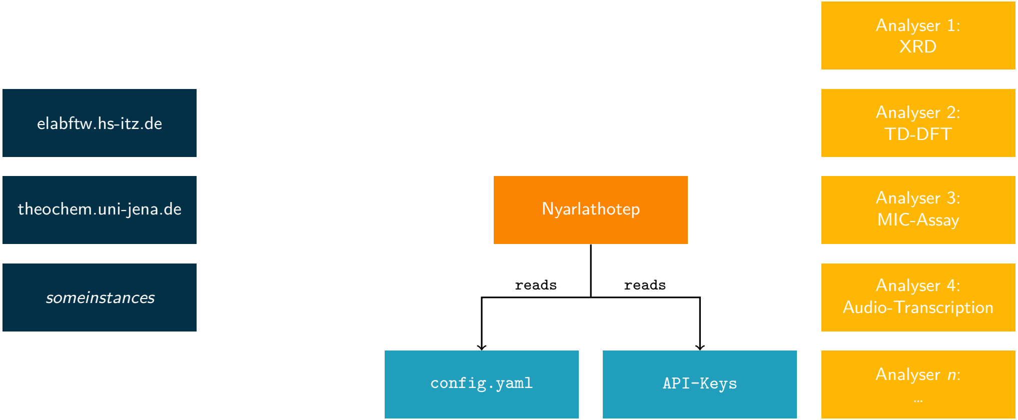

elabftw.hs-itz.de

theochem.uni-jena.de

someinstances

Nyarlathotep

`config.yaml`

`API-Keys`

Analyser 1: XRD

Analyser 2: TD-DFT

Analyser 3: MIC-Assay

Analyser 4: Audio-Transcription

Analyser *n*: ...

Components

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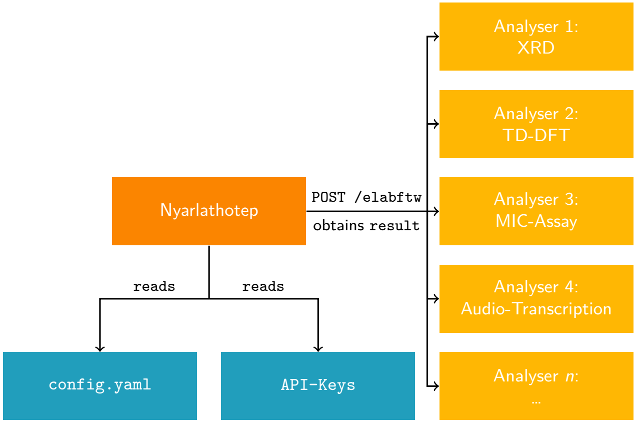
theochem.uni-jena.de

someinstances



Nyarlathotep

`POST /elabftw`

`obtains result`

`reads`

`reads`

`config.yaml`

`API-Keys`

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Analyser 3: MIC-Assay

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Analyser *n*: ...

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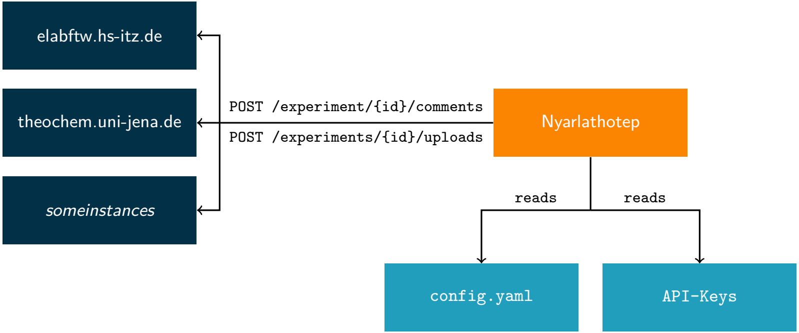
elabftw.hs-itz.de
theochem.uni-jena.de
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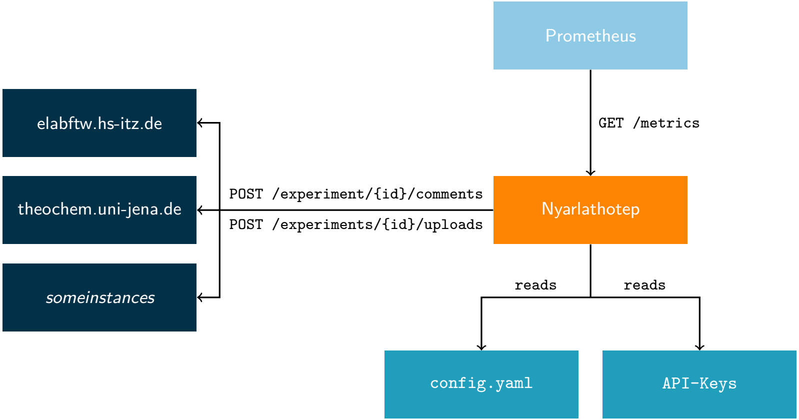

Prometheus
GET /metrics
elabftw.hs-itz.de
theochem.uni-jena.de
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Generating Clients

- Nyarlathotep generates current API specification for workers

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nyarlathotep print worker >
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Generating Clients

- Nyarlathotep generates current API specification for workers
- Generate client's server via OpenAPI generator
- Hook up your processing code to the server endpoints

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Generating Clients

Connect server and analysis code

```
main :: IO ()
main = do
  -- ...
  runWorkerServer (Config cfgUrl) . Worker $ workerFn

-- | Wrapping and unwrapping request and result types from JSON
workerFn :: (MonadIO m) => WorkerRequest -> m WorkerResults
workerFn WorkerRequest{..} = do
  (tempF, volF, denF) <- run workDir equiF prodF
  return $ WorkerResults { ... }

-- | Your normal analysis code without any specialties
run :: MonadIO m => FilePath -> FilePath -> FilePath -> m (FilePath,
    FilePath, FilePath)
```

Scenarios

Central Instance, e.g. compute centre

- Runs Nyarlathotep and workers on Kubernetes cluster

Local instance, e.g. per Workgroup

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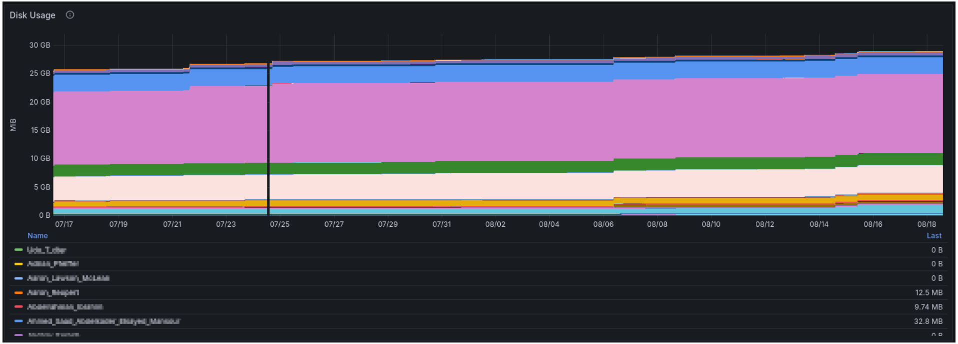
- Local group admin and/or users can add workflows themselves

Monitoring

- Nyarlathotep provides OpenMetrics endpoint
- Disk usage per user from the `/reports` API
- Statistics on processed experiments, e.g. processing time, success and failure rates



Name	Last
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[redacted]	0 B
[redacted]	12.5 MB
[redacted]	9.74 MB
[redacted]	32.8 MB
[redacted]	0 B

Outlook & Conclusion

- Nyarlathotep is in an early stage and still changes
- Our use case: collect data for chemical compounds, normalise them and build up an external ML database
- Standardise workflows for common measurements

https://git.uni-jena.de/mi24ris/nyarlathotep