



LatteDB (*in development*)

— Database oriented workflow management (for LQCD)

In collaboration with Jason Chang and



Christopher Körber | UC Berkeley | Feodor Lynen Fellow



Unterstützt von / Supported by



Alexander von Humboldt
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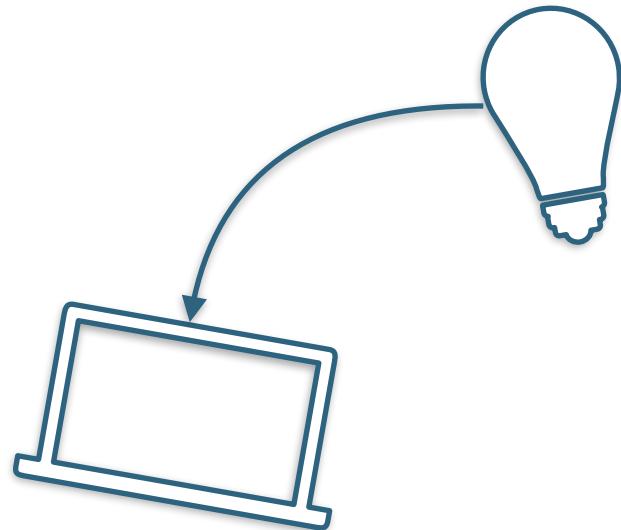
Workflow

- **Scientific Idea**
 - Specification of problem
 - Feasibility studies



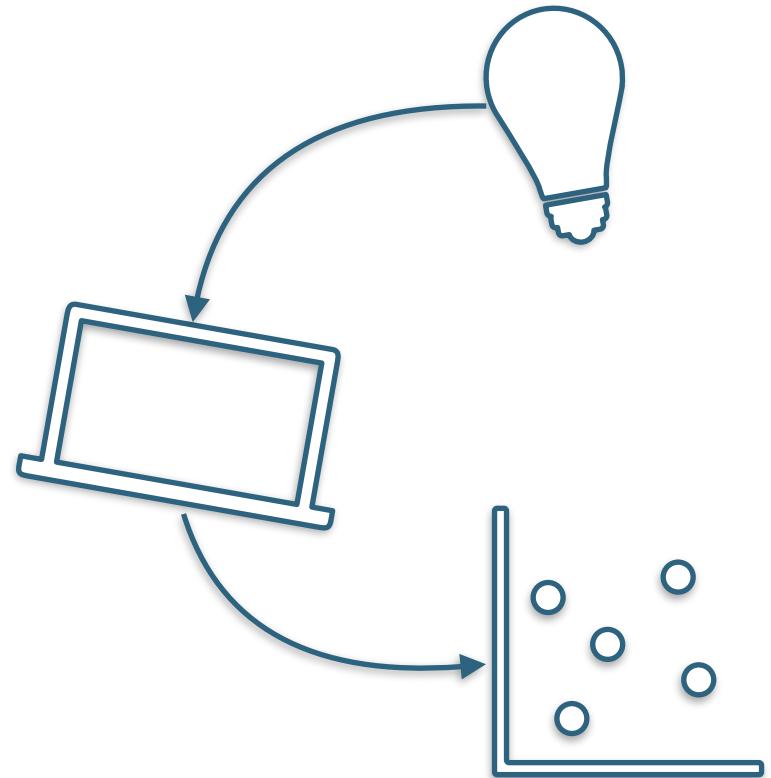
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- **Code Development**
 - Creating new code
 - Optimizing old code
- **Computation**
 - Job allocation & monitoring



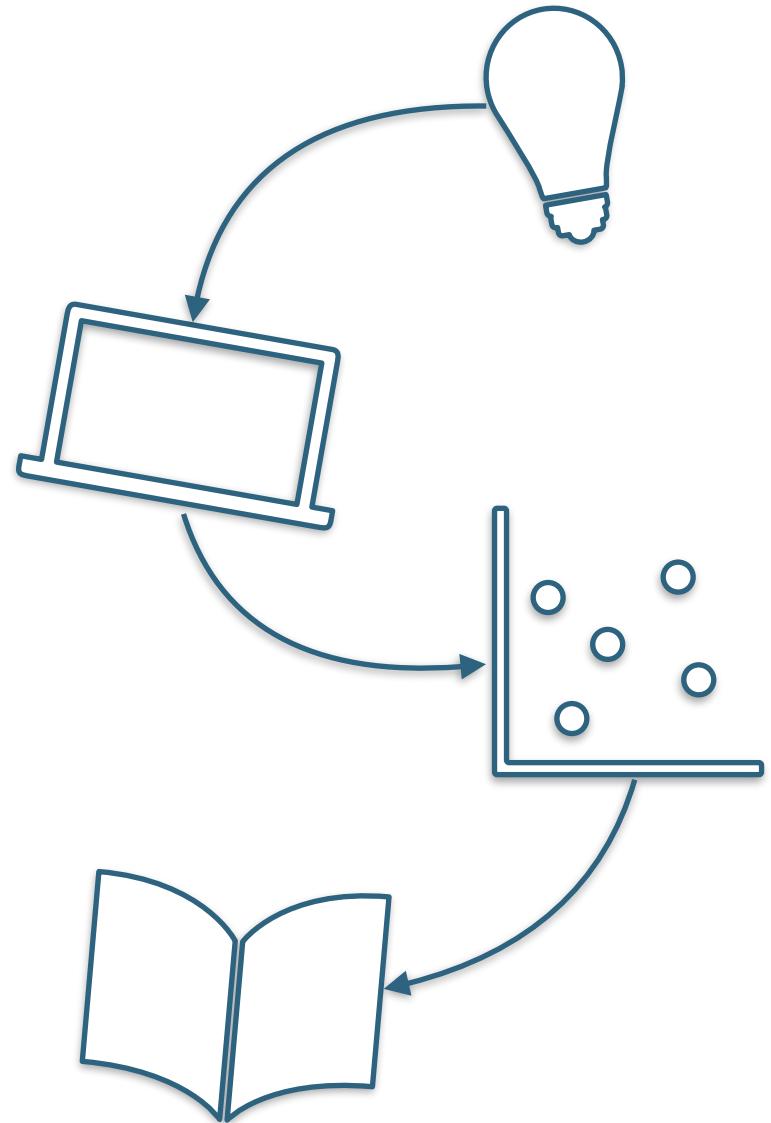
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 - Collecting files
 - Extracting relevant information



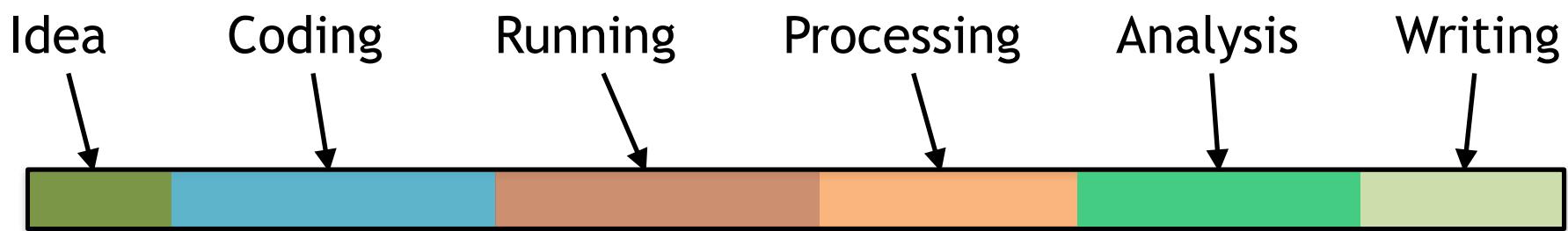
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- **Analysis**
- **Writing Publication**



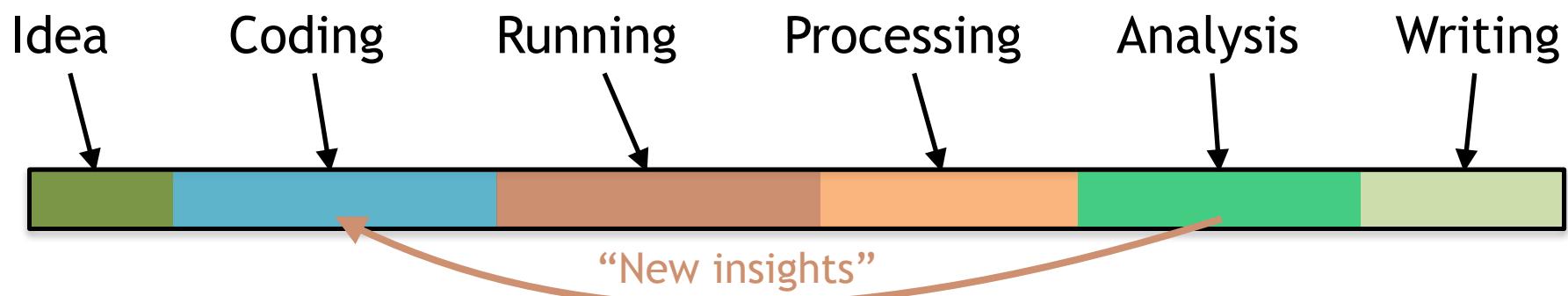
Time scales

~ Rough average estimation



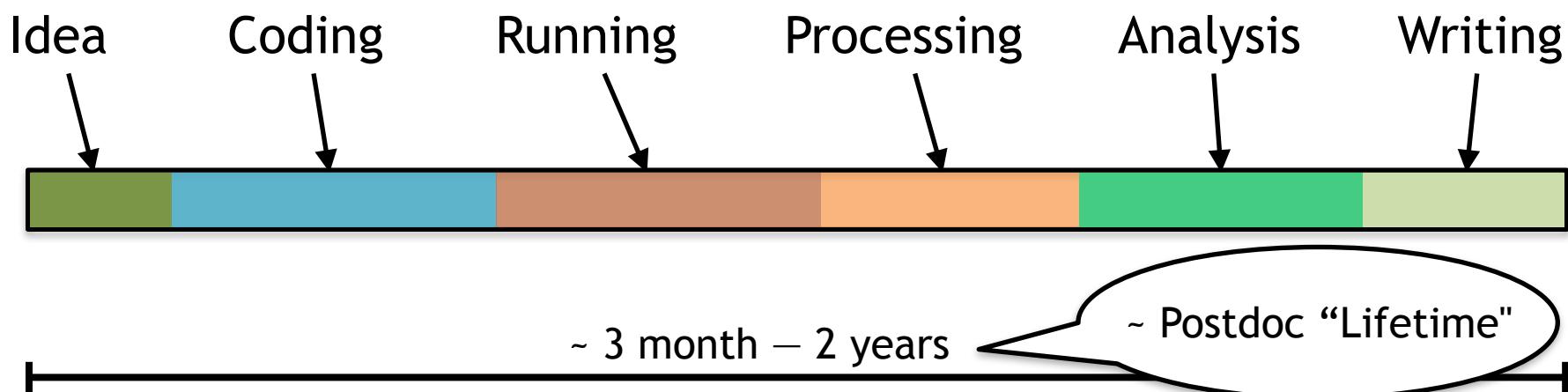
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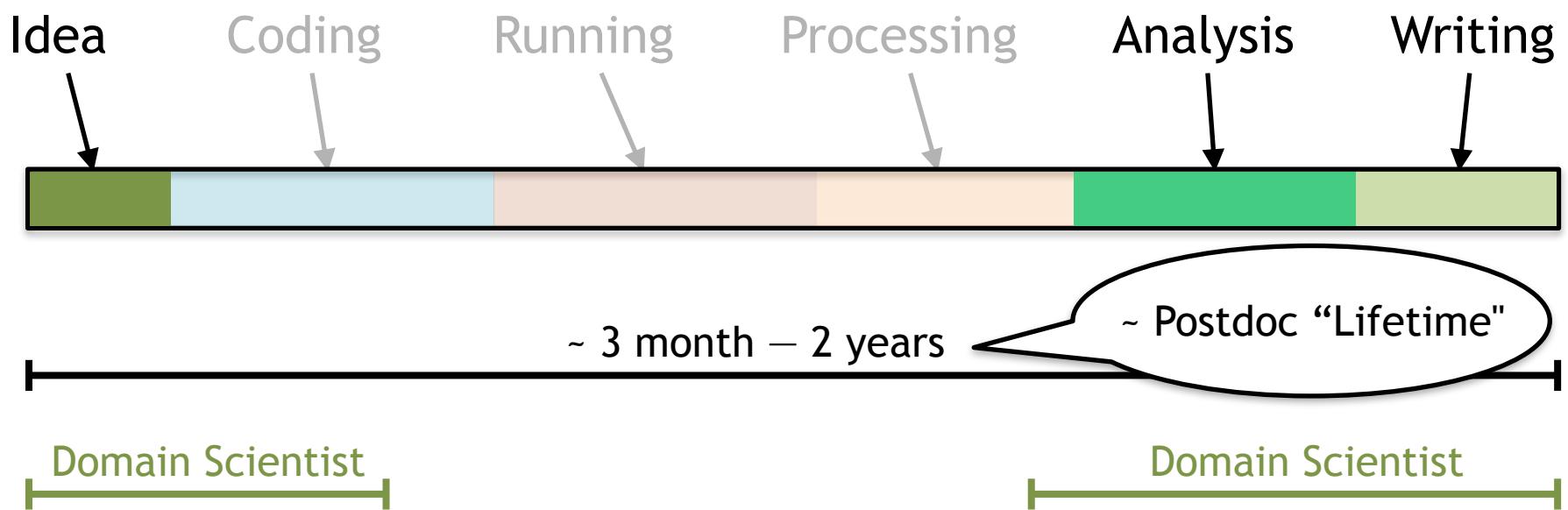
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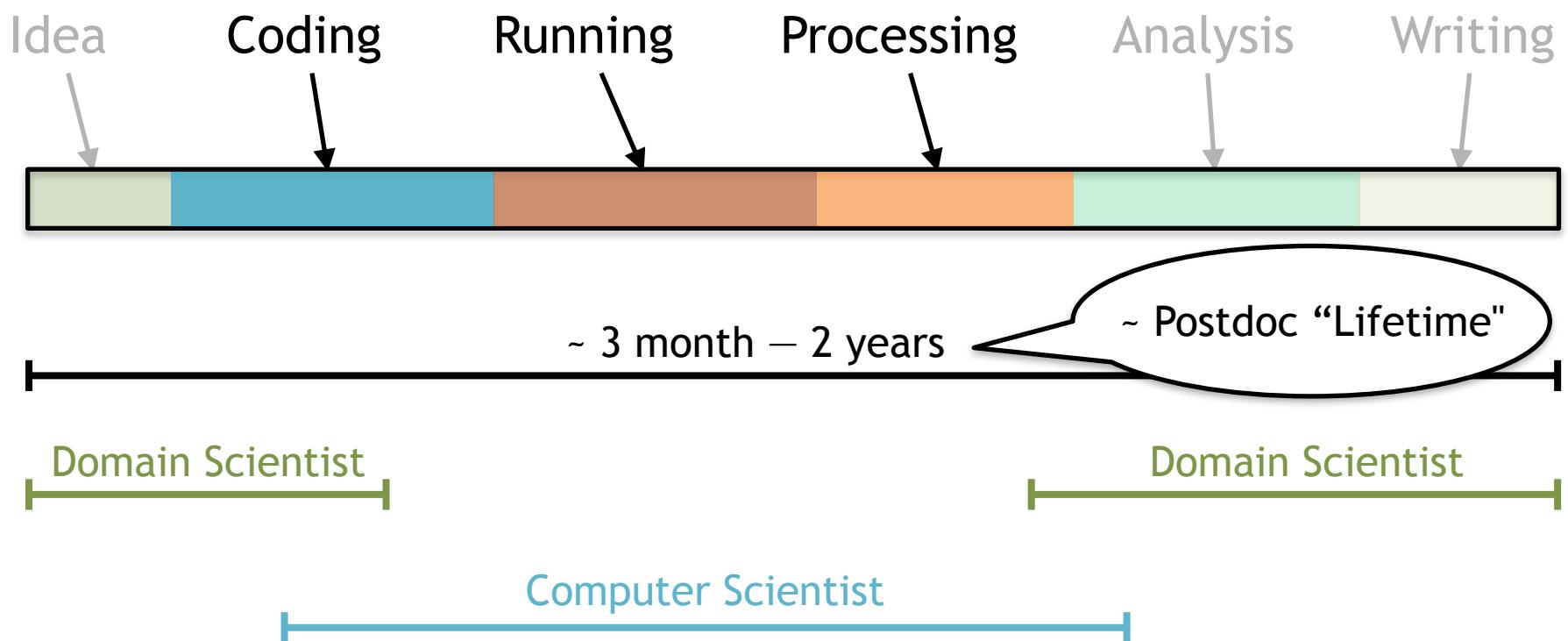
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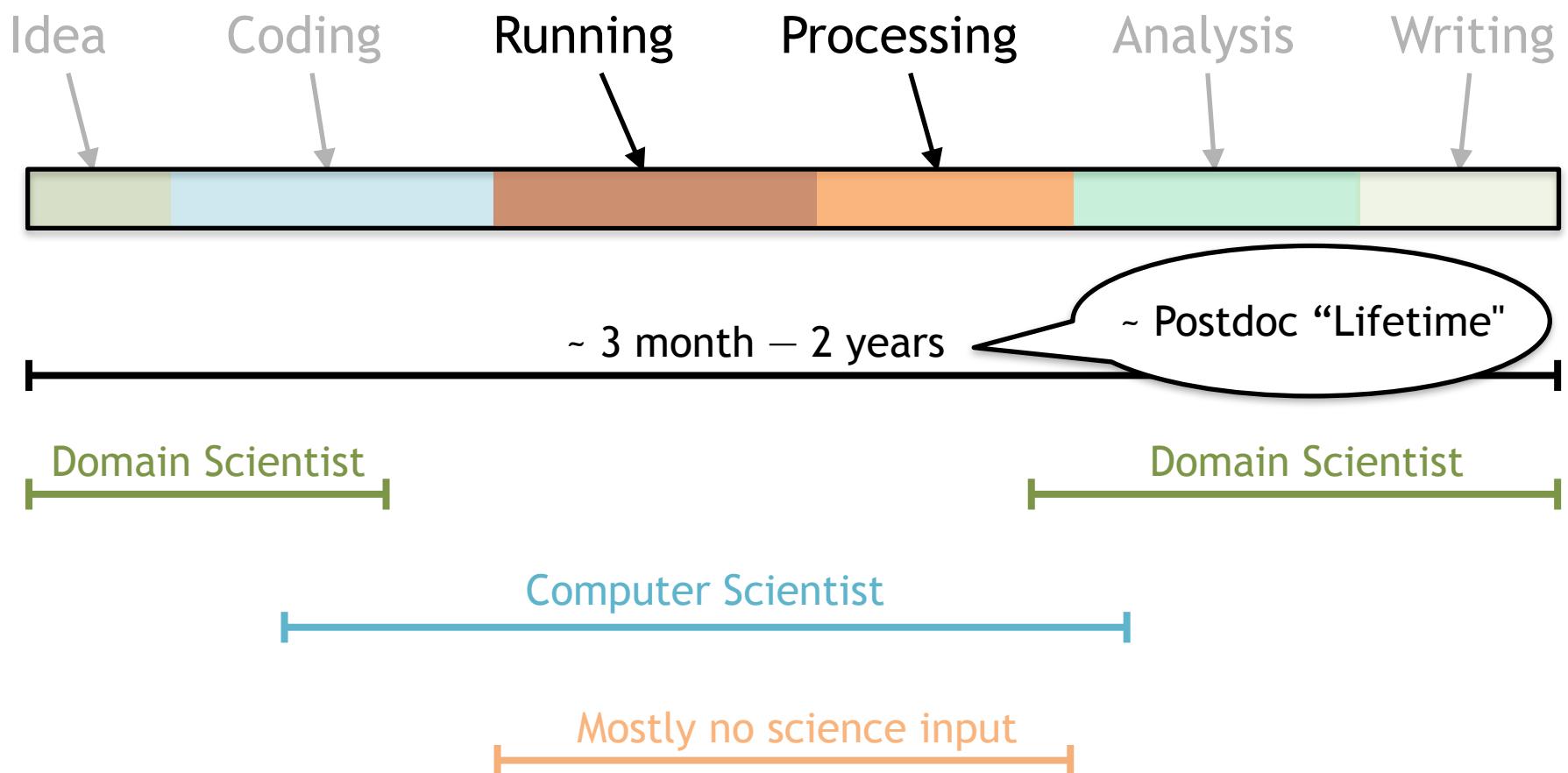
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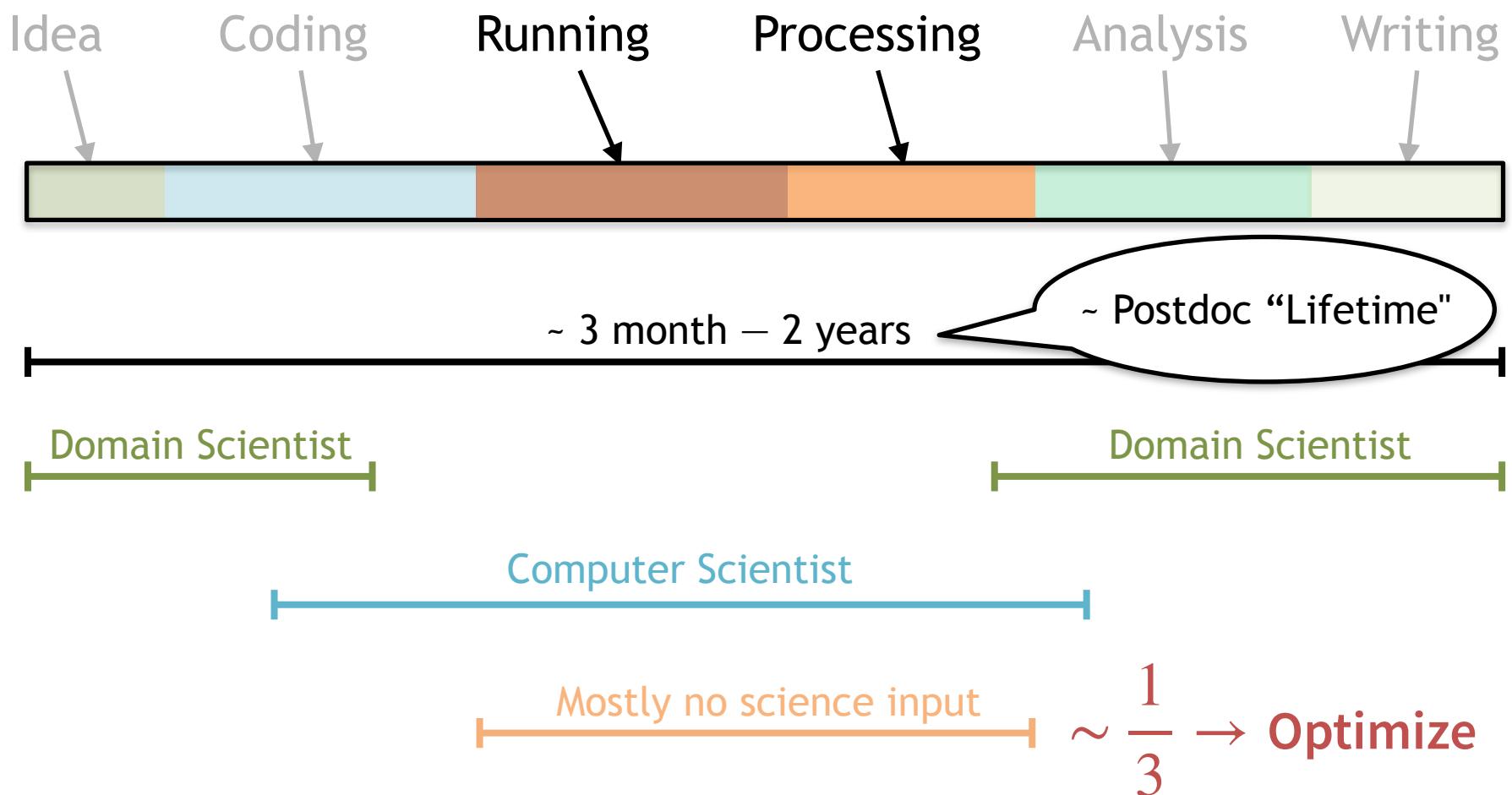
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Overview

→ We have many files...

- **Computation [1,2]**

- Job generation → large physics & computation parameter space
- Job scheduling → bundle jobs to large allocation
 - Computation requirements (GPU vs CPU)
 - Dependencies requirements (A → B)
 - Job manager based on (many) job files

- [1] github.com/evanberkowitz/metaq
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- [3] github.com/callat-qcd/nucleon_elastic_FF
- [4] github.com/callat-qcd/project_gA

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 - Raw data ~ several hundred terabytes (many data files)
 - Transform data to analysis
 - Averaging, Fourier transforming, concatenating, resampling, ...

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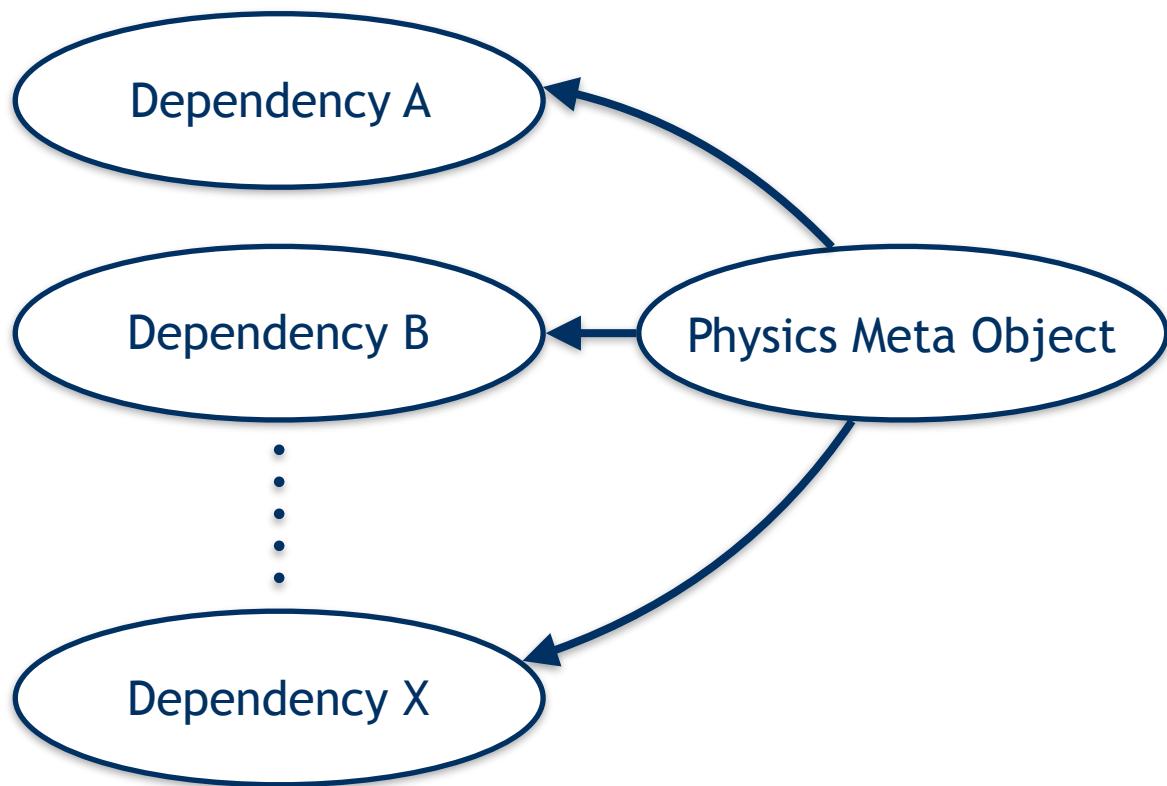
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- **Data Post-Processing [3]**
 - Raw data ~ several hundred terabytes (many data files)
 - Transform data to analysis
 - Averaging, Fourier transforming, concatenating, resampling, ...
- **Analysis [4]**
 - Statistical data → Physical parameters
 - Input data, fit models → results & uncertainties

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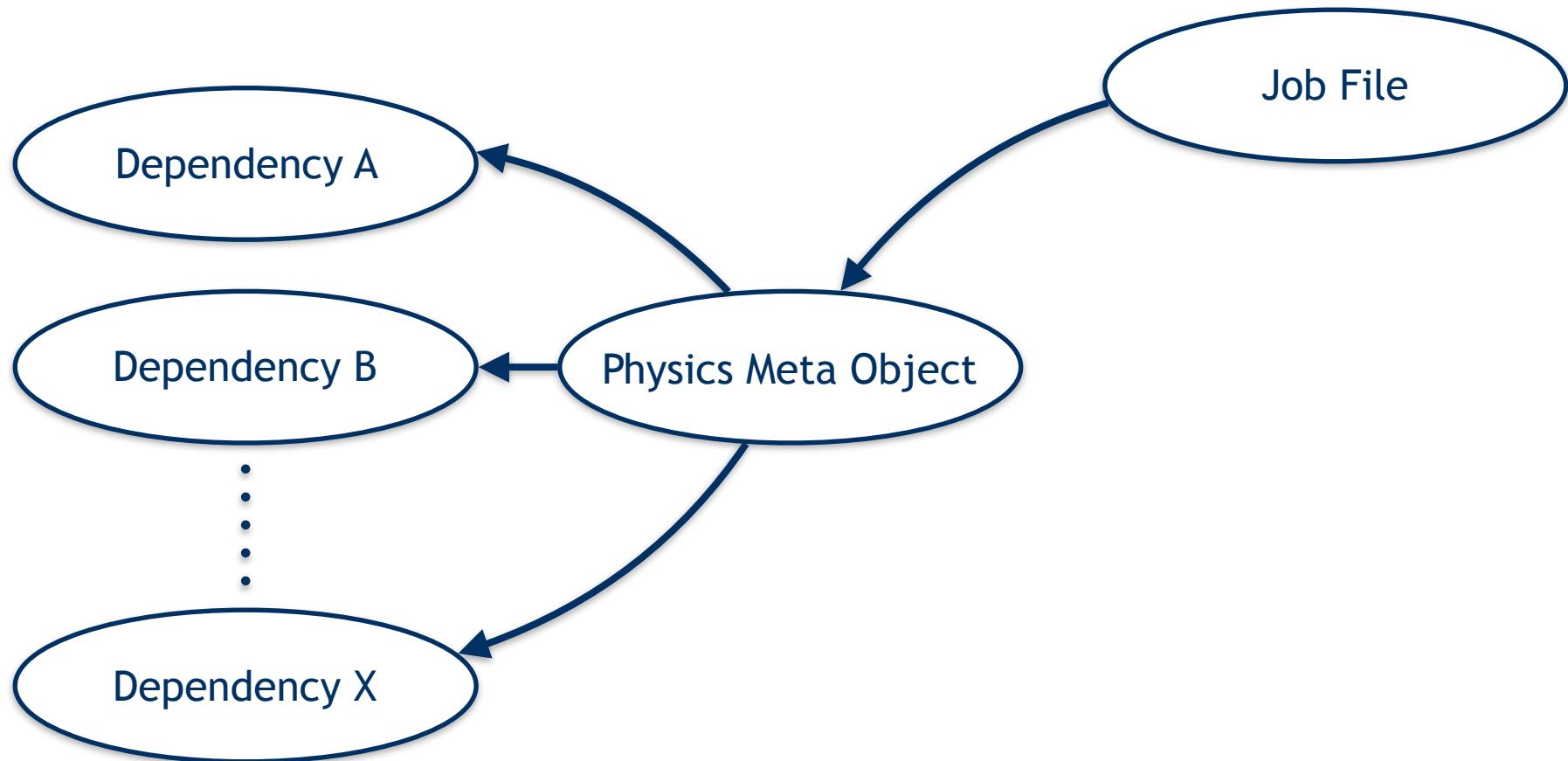
Abstraction:

→ Workflow controlled by physics meta objects



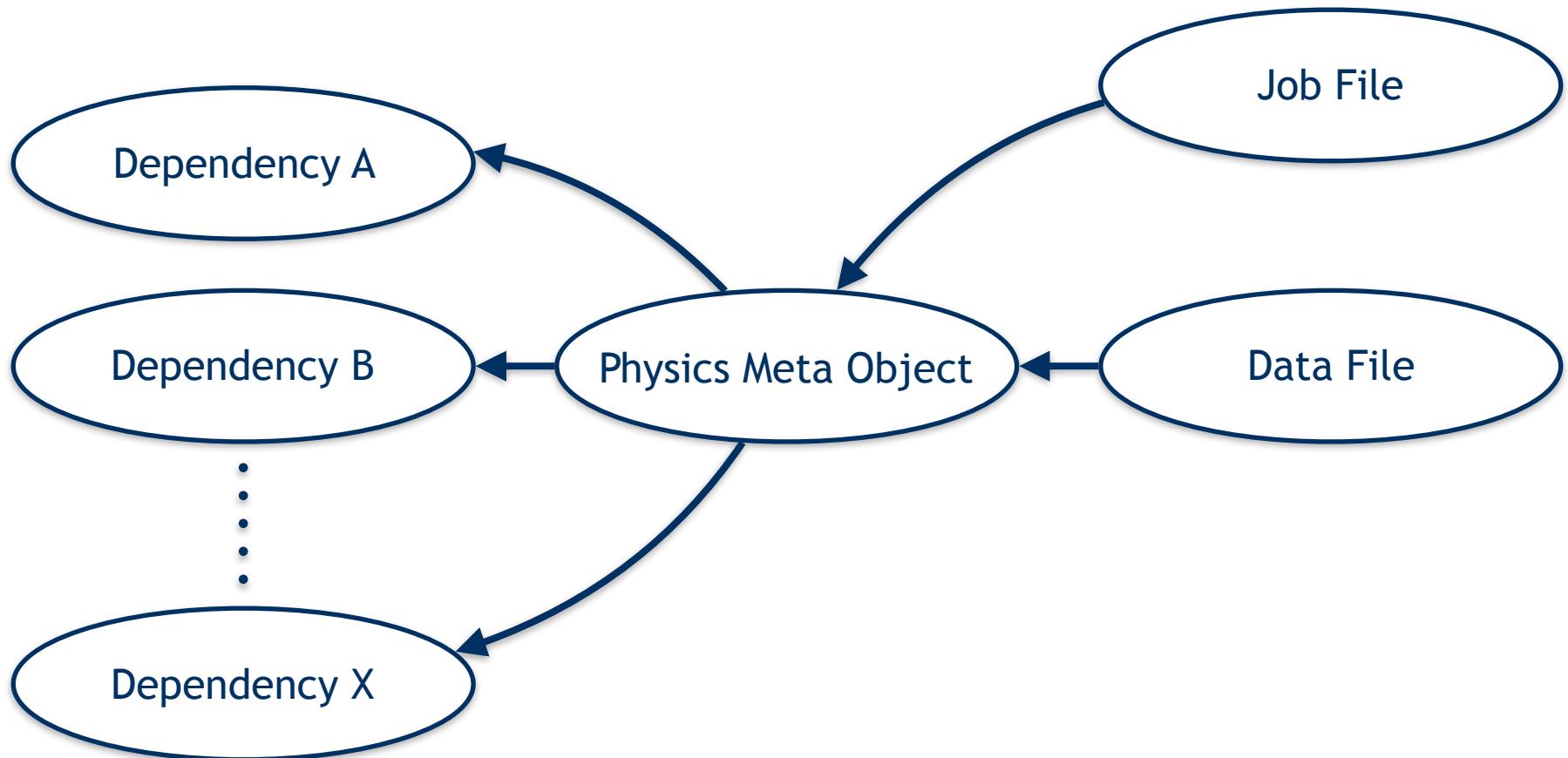
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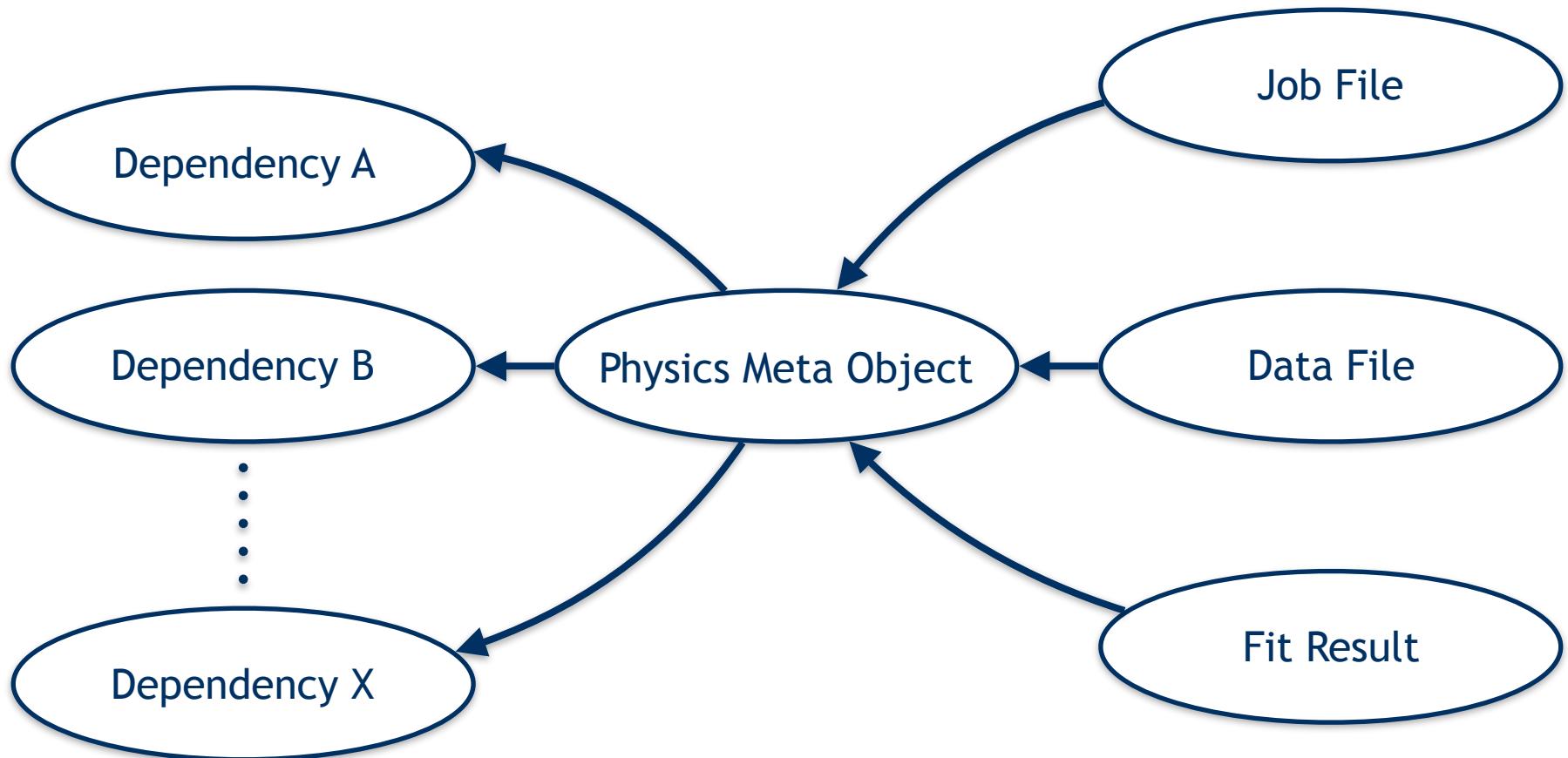
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Idea

→ Replace: file based approach → DataBaseBased approach

- First Order Advantages of Database
 - Systemic storage of data
 - no string parsing required (regex)

```
300/prop_a09m310_e_300_gf1.0_w3.5..._x3y3z19t62.lime
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- First Order Advantages of Database
 - Systemic storage of data
 - no string parsing required (regex)
 - Relationship between data
 - $A \rightarrow B$

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vs

propagator_ptr_id	origin_x	origin_y	origin_z	origin_t	fermionaction_id
1	2	2	14	31	4
2	14	14	2	31	4
3	16	23	18	7	4

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- Filtering of data
 - Fast & automatic status repo

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pattern = r"..._x(?P<x>[0-9]+)...lime"
for file in propagator_files:
    if re.match(pattern, file) and ...:
        filterd_files.append(file)
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VS

```
SELECT * FROM Propagator WHERE origin_x > 3;
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- Convince group to use database
 - “Learning of language SQL”

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- **First Order Challenges**

- Convince group to use database
 - “Learning of language SQL”
- Map existing system to new structure
 - “Never change a running system”

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Framework

[1] www.djangoproject.com

→ Django: "The web framework for perfectionists with deadlines" [1]

Object–Relational Mapper (ORM)

- Maps database tables to Python objects
 - Users don't have to learn SQL
 - Integrates easily in existing code

Framework

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Django

- Well maintained
 - Used by: Pinterest, Instagram, Bitbucket, Mozilla Support, ...
- Well documented
 - Tutorials, multiple version history, multiple languages, ...
- Open Source
 - Active development, many extensions, ...

Python Classes ↔ Tables

Nf211(GaugeConfig) Table

	SHORT TAG	STREAM	CONFIG	NX	NY	NZ	NT	MPI
□	a09m310	e	396	32	32	32	96	310.000000
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2nd Order Advantages:

- Consistency checks
- Auto-documentation
- High-level API support

Object Relational Manager
converts SQL to class

Convert all rows (lazy)

Check/adjust status of configs

Insert/Update database

Relationships & Updates

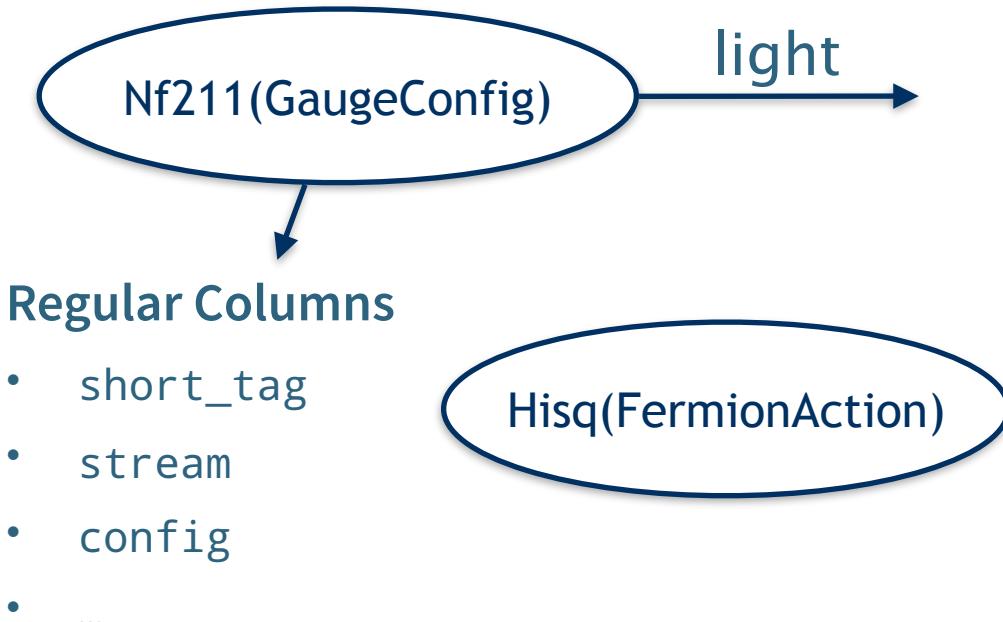


Regular Columns

- short_tag
- stream
- config
- ...

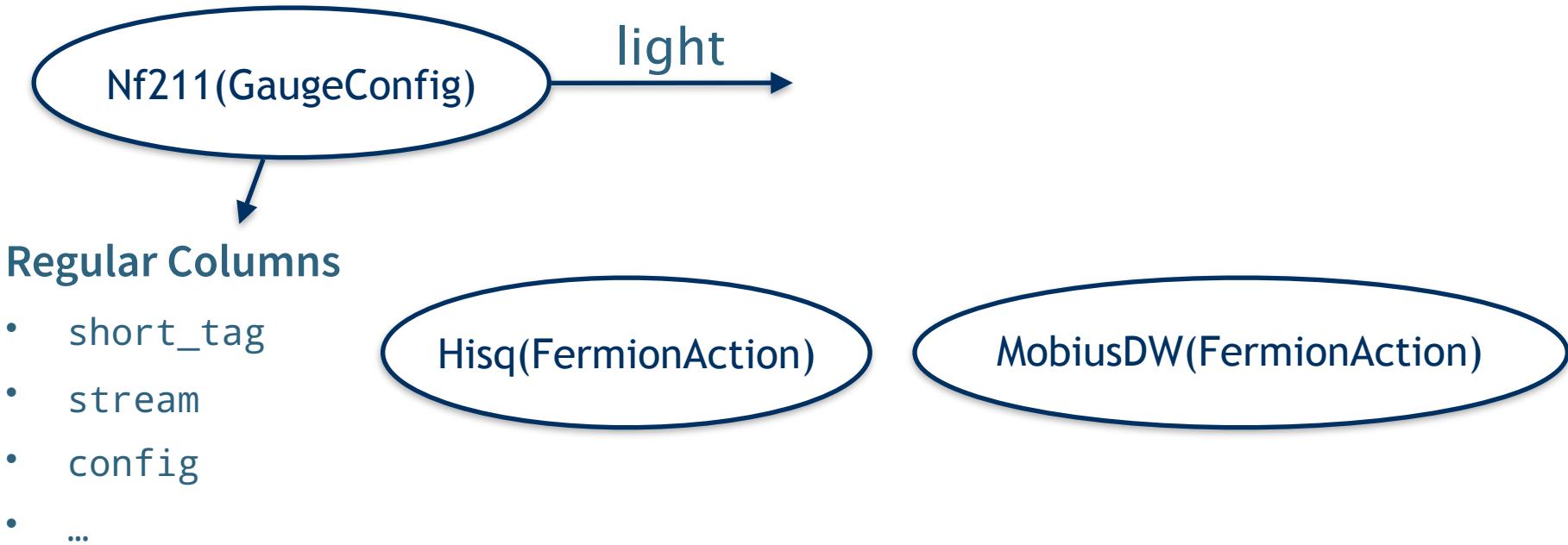
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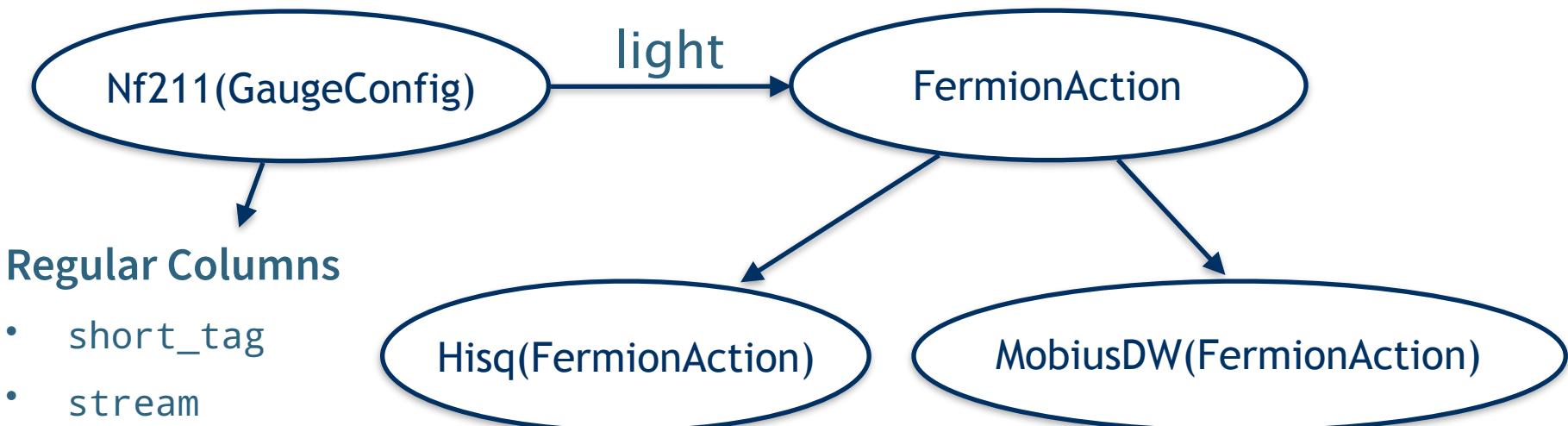
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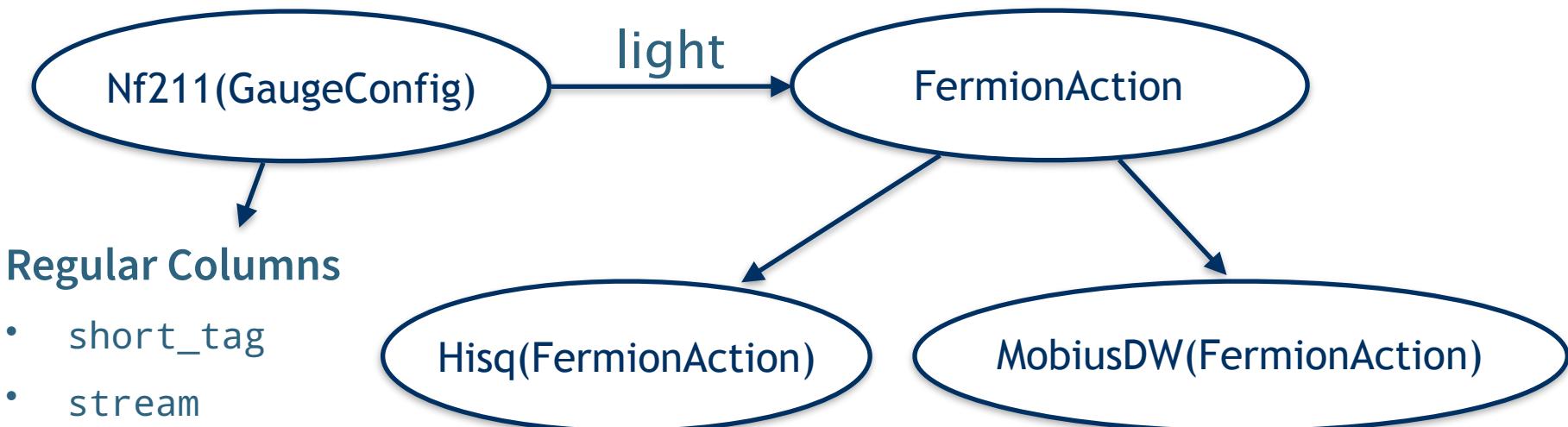
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- short_tag
- stream
- config
- ...

Relationships & Updates

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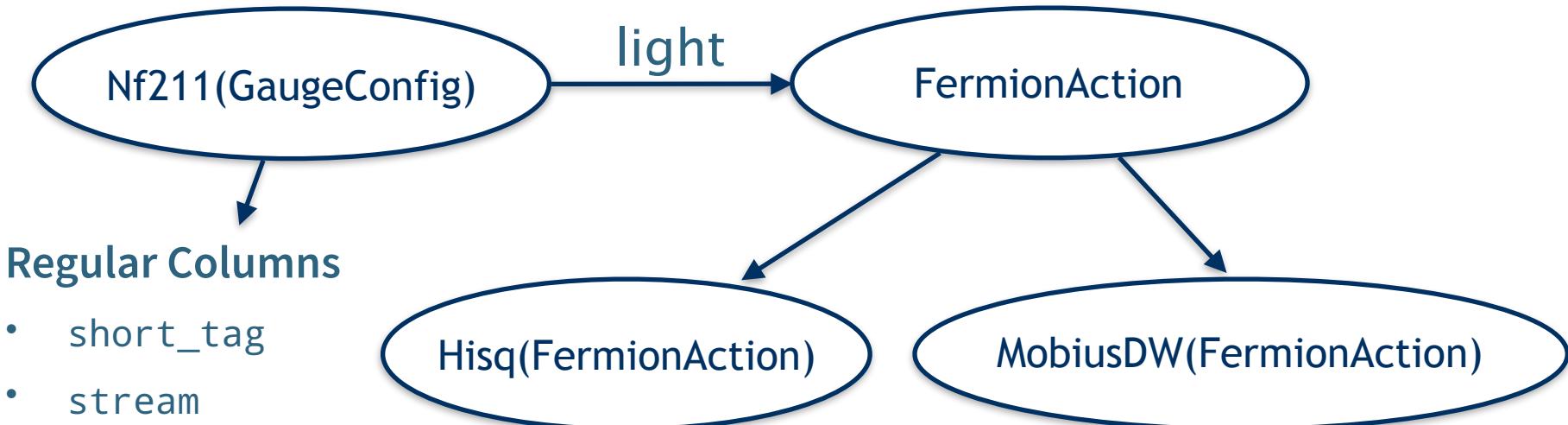


- `short_tag`
- `stream`
- `config`
- ...

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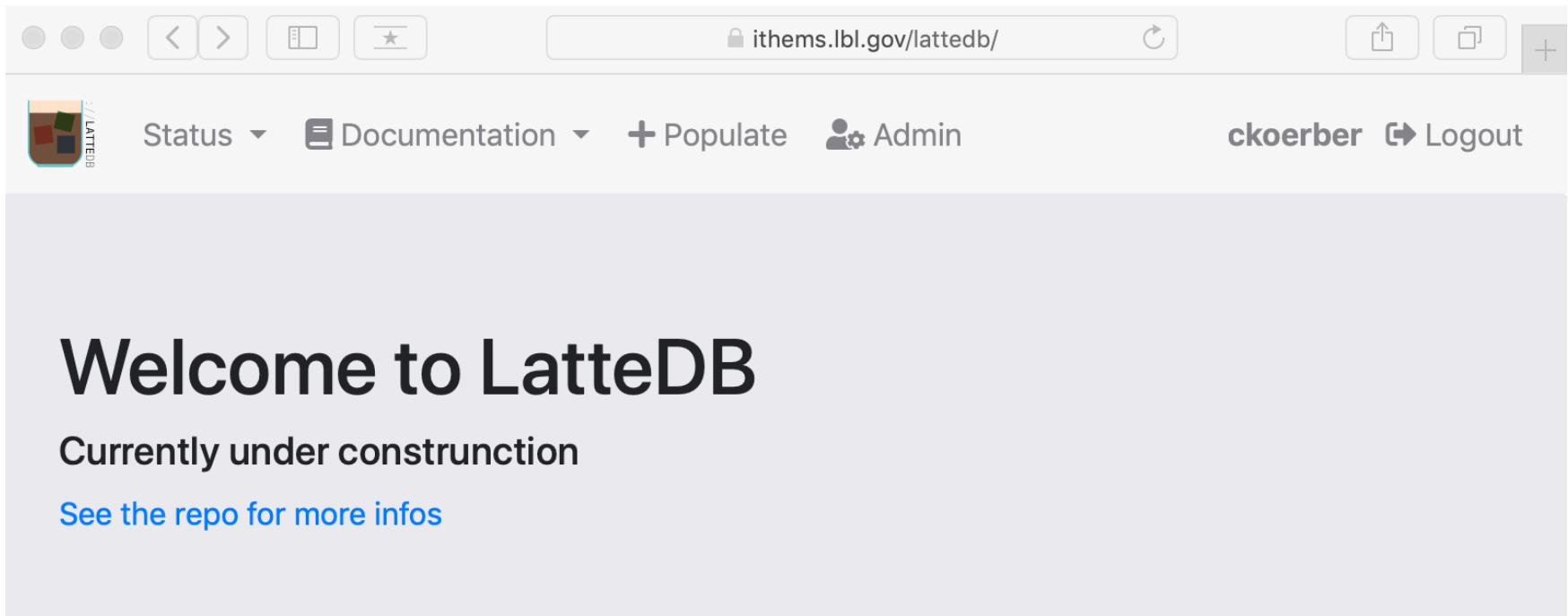


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2nd Order Advantages:

- Information reuse
- Flexibility

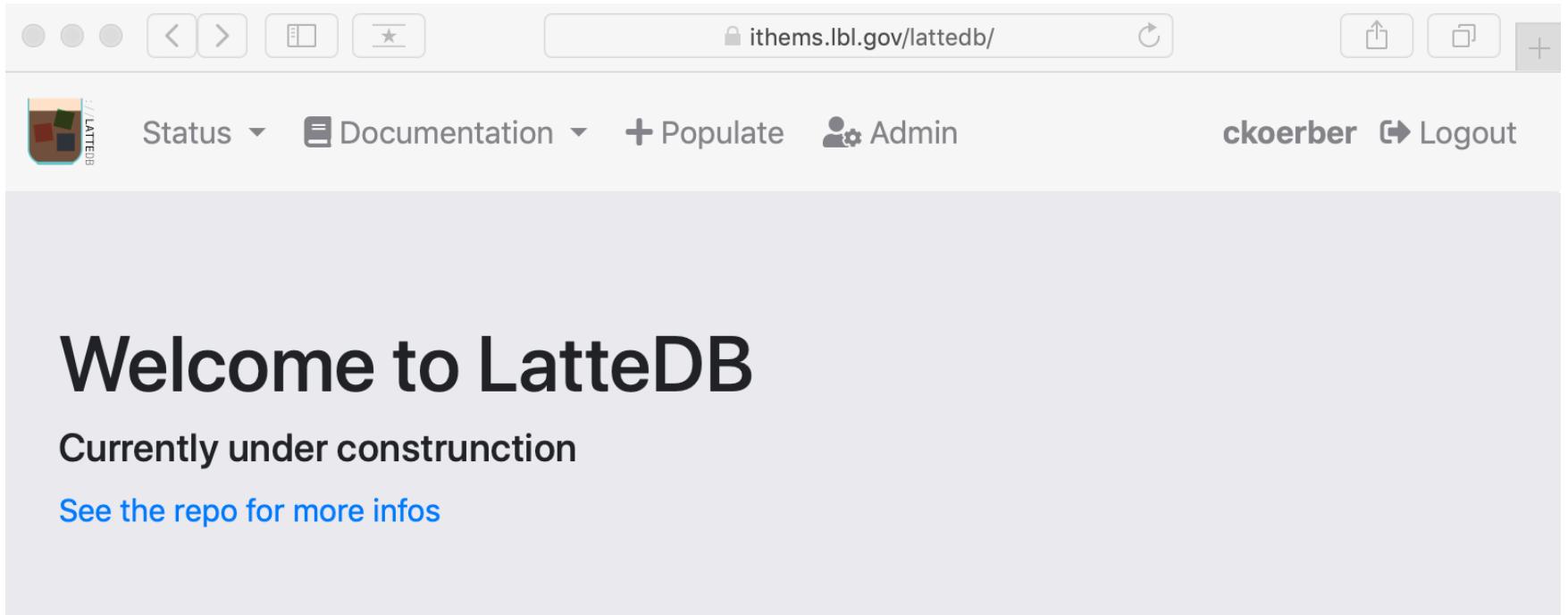
Features: Webpage



The screenshot shows a web browser window with the following details:

- Address Bar:** ithems.lbl.gov/lattedb/
- Header:** A navigation bar with icons for back, forward, search, and refresh.
- User Profile:** ckoerber Logout
- Page Content:**
 - A logo icon with the text ":// LATTEDB".
 - Navigation links: Status, Documentation, Populate, Admin.
 - Welcome message: "Welcome to LatteDB".
 - Status message: "Currently under construction".
 - Info link: "See the repo for more infos".

Features: Webpage



The screenshot shows a web browser window with the URL `ithems.lbl.gov/lattedb/` in the address bar. The page itself is titled "Welcome to LatteDB" and contains the message "Currently under construction". It also includes a link "See the repo for more infos". The top navigation bar includes links for "Status", "Documentation", "Populate", "Admin", and user information "ckoerber" with a "Logout" button. The browser's standard header with back/forward buttons and a search bar is visible at the top.

2nd Order Advantages:

- Automated progress reports
- Centralized source for information
- Easy to set up open data platform

Features: Table views

Real view – fake data

Home > Correlator > Baryon2pts

Select baryon2pt to view

Action:	ID	ENSEMBLE	CONFIG	TAG	ORIGIN (X, Y, Z, T)	PARITY	SPIN X2	SPIN Z X2	ISOSPIN X2	ISOSPIN Z X2
<input type="checkbox"/>	1888	a09m310	396	proton	(7, 29, 23, 41)	1	1	1	1	1
<input type="checkbox"/>	1887	a09m310	396	proton	(7, 29, 23, 41)	1	1	-1	1	1
<input type="checkbox"/>	1886	a09m310	396	proton	(7, 29, 23, 41)	-1	1	1	1	1
<input type="checkbox"/>	1885	a09m310	396	proton	(7, 29, 23, 41)	-1	1	-1	1	1
<input type="checkbox"/>	1884	a09m310	396	proton	(23, 13, 7, 41)	1	1	1	1	1
<input type="checkbox"/>	1883	a09m310	396	proton	(23, 13, 7, 41)	1	1	-1	1	1
<input type="checkbox"/>	1882	a09m310	396	proton	(23, 13, 7, 41)	-1	1	1	1	1
<input type="checkbox"/>	1881	a09m310	396	proton	(23, 13, 7, 41)	-1	1	-1	1	1
<input type="checkbox"/>	1880	a09m310	396	proton	(18, 21, 25, 89)	1	1	1	1	1
<input type="checkbox"/>	1879	a09m310	396	proton	(18, 21, 25, 89)	1	1	-1	1	1

FILTER

By tag

All
proton

By ensemble

All
a15m310L
a09m310
a12m310

Features: Automatic Progress Report

Baryon2pt Status progress view

Real view – fake data

Listed by Ensemble

a12m310 I2464f211b600m010m050m635

Progress (total=672)

Does not exist: 81 Unknown: 81 On tape: 243 On filesystem: 267

a15m310L I2448f211b580m013m065m838

Progress (total=672)

Does not exist: 74 Unknown: 71 On tape: 261 On filesystem: 266

a09m310 I3296f211b630m007m037m440

Progress (total=544)

Does not exist: 78 Unknown: 55 On tape: 208 On filesystem: 203

Features: Automatic Documentation

Documentation of `lattedb.propagator`

See table properties

`OneToAll`

Module: `lattedb.propagator.models`

Base: `Propagator[Base]`

Columns

Name	Type	Help
<code>tag</code>	<code>CharField</code> (Optional)	(Optional) Char(20): User defined tag for easy searches
<code>misc</code>	<code>JSONField</code> (Optional)	(Optional) JSON: {'anything': 'you want'}
<code>gaugeconfig</code>	<code>ForeignKey: GaugeConfig</code>	ForeignKey pointing to specific gauge configuration inverted on
<code>fermionaction</code>	<code>ForeignKey: FermionAction</code>	ForeignKey pointing to valence lattice fermion action
<code>origin_x</code>	<code>PositiveSmallIntegerField</code>	PositiveSmallInt: x-coordinate origin location of the propagator
<code>origin_y</code>	<code>PositiveSmallIntegerField</code>	PositiveSmallInt: y-coordinate origin location of the propagator
<code>origin_z</code>	<code>PositiveSmallIntegerField</code>	PositiveSmallInt: z-coordinate origin location of the propagator
<code>origin_t</code>	<code>PositiveSmallIntegerField</code>	PositiveSmallInt: t-coordinate origin location of the propagator

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> touch new_app/models.py  
> lattedb makemigrations  
> lattedb migrate
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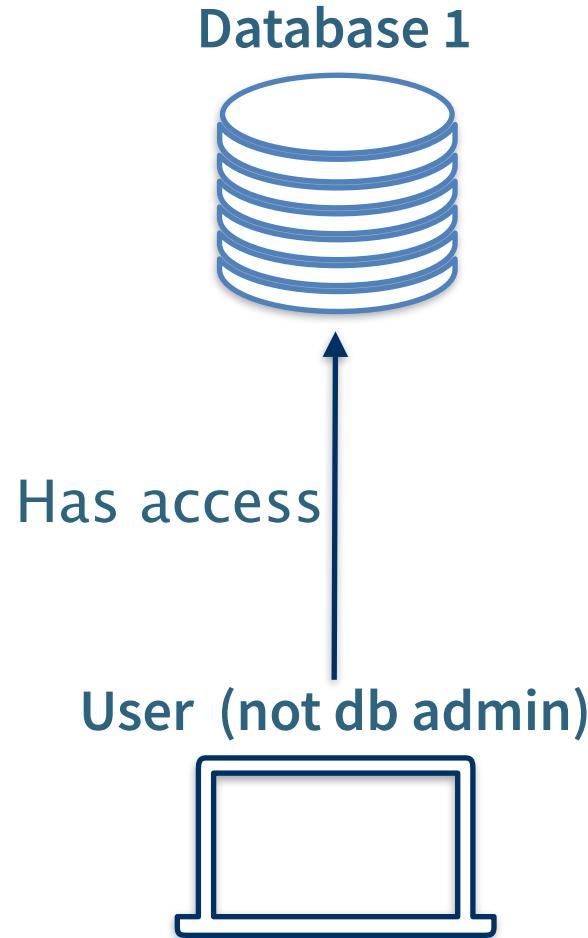
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1 from lattedb.propagator.models import OneToMany
```

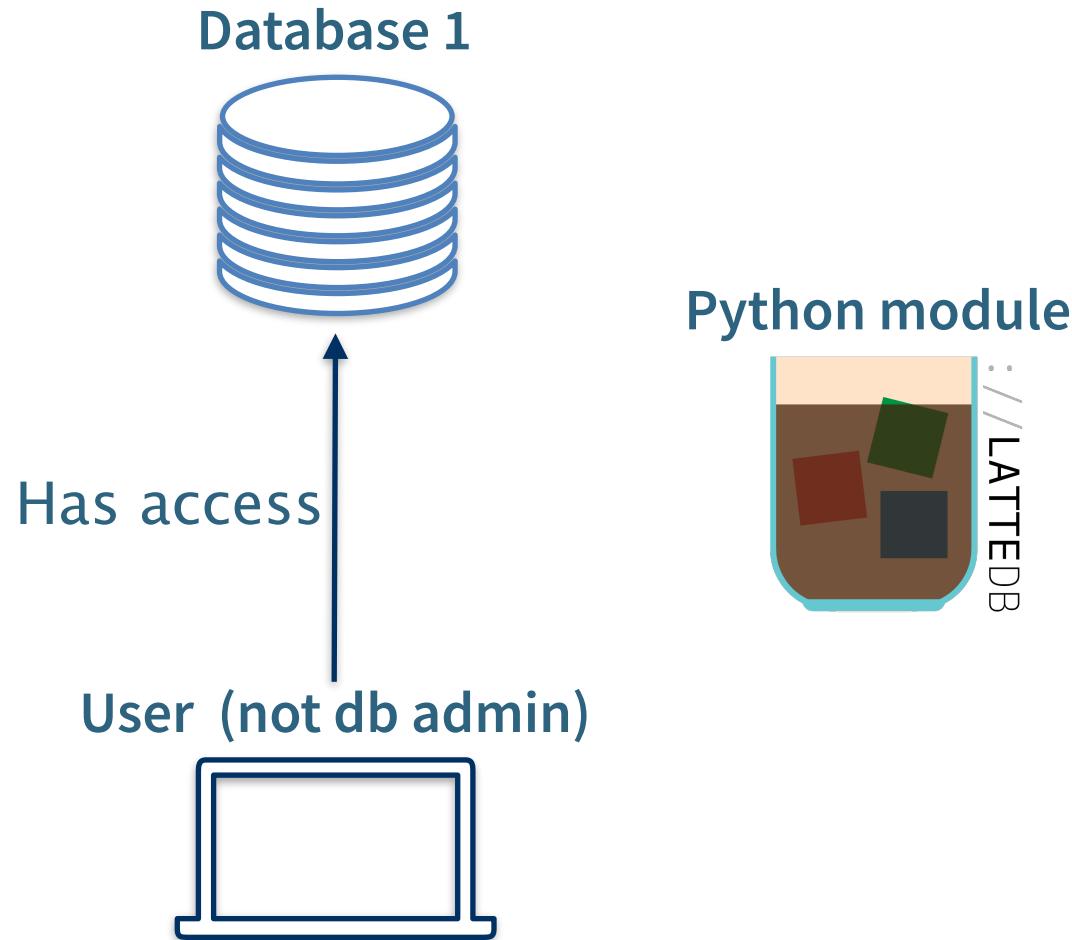
7. launch the webapp (on localhost)

```
> lattedb runserver
```

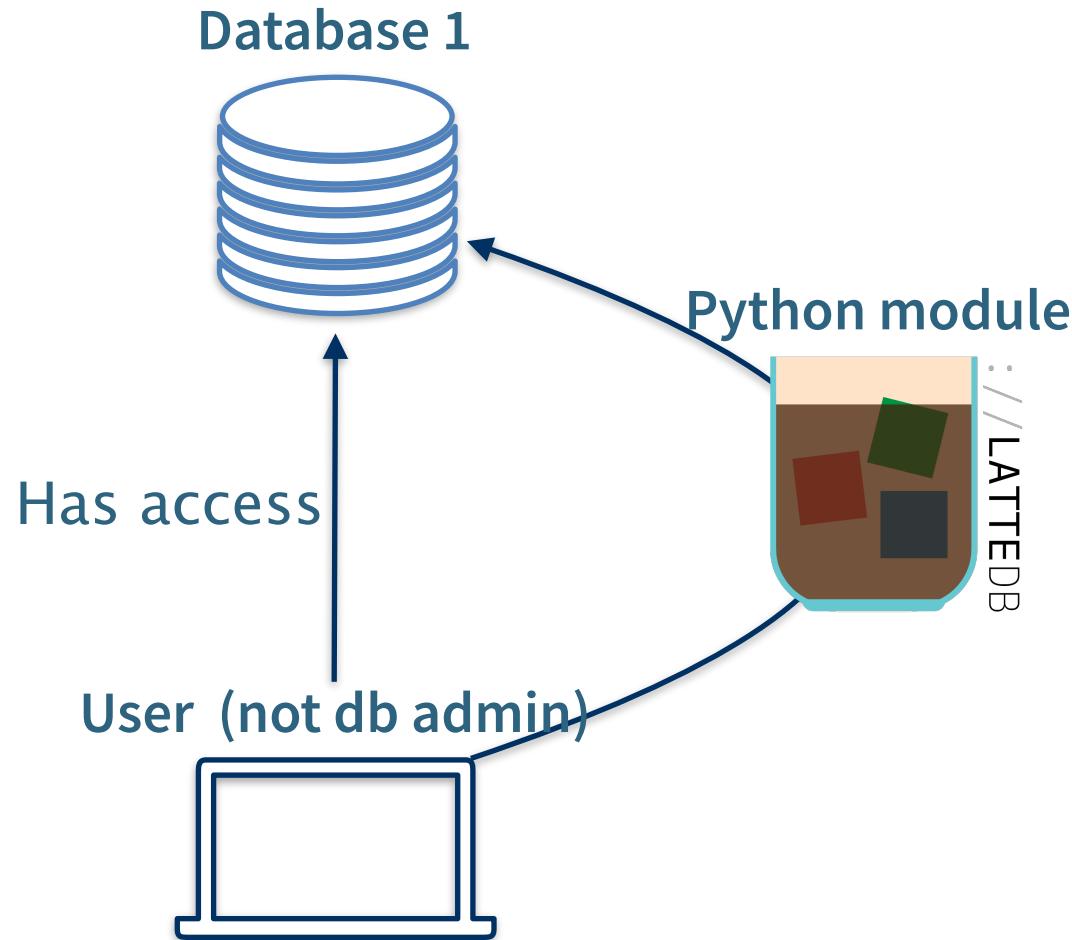
Security Layers (Python Module)



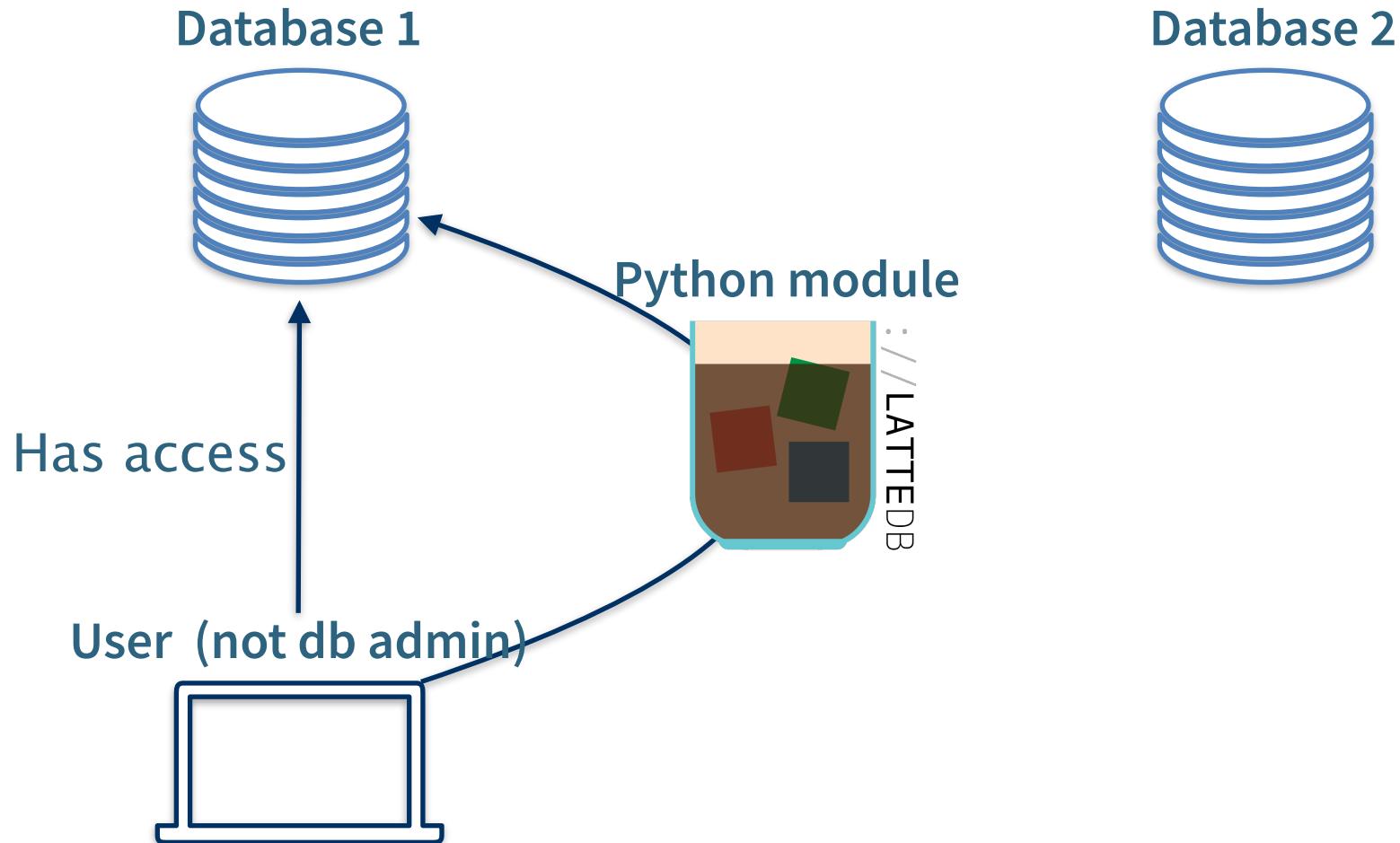
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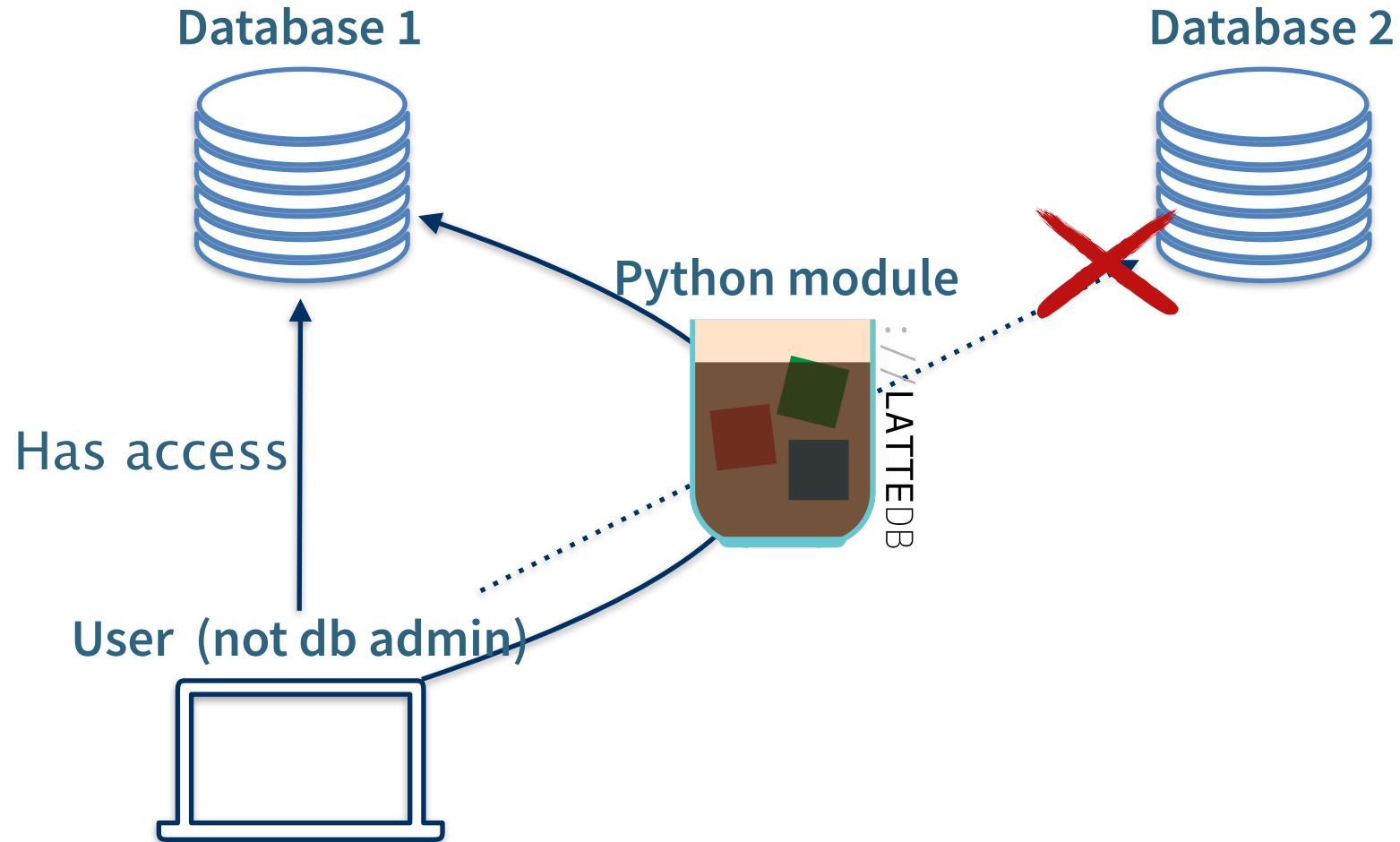
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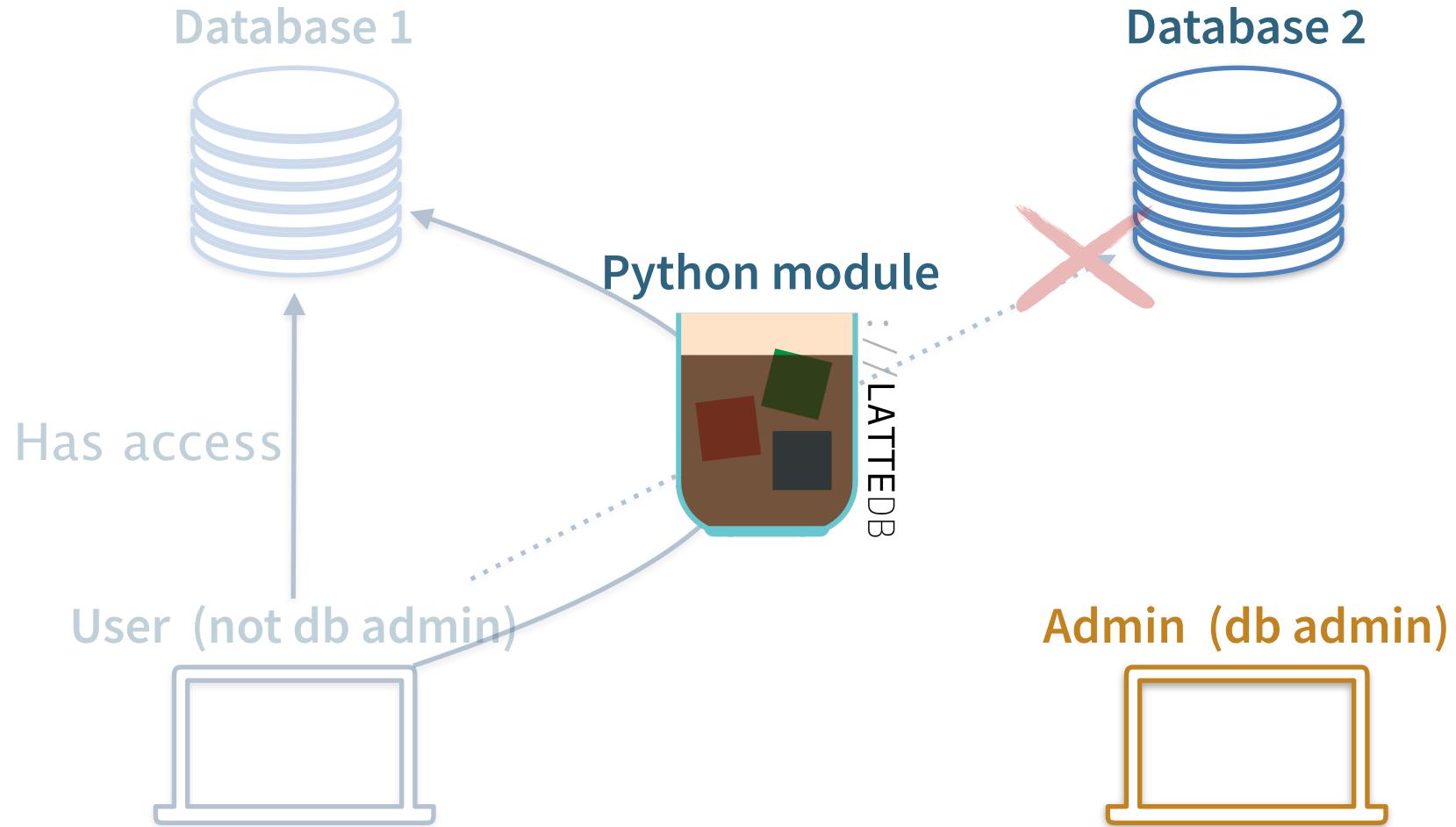
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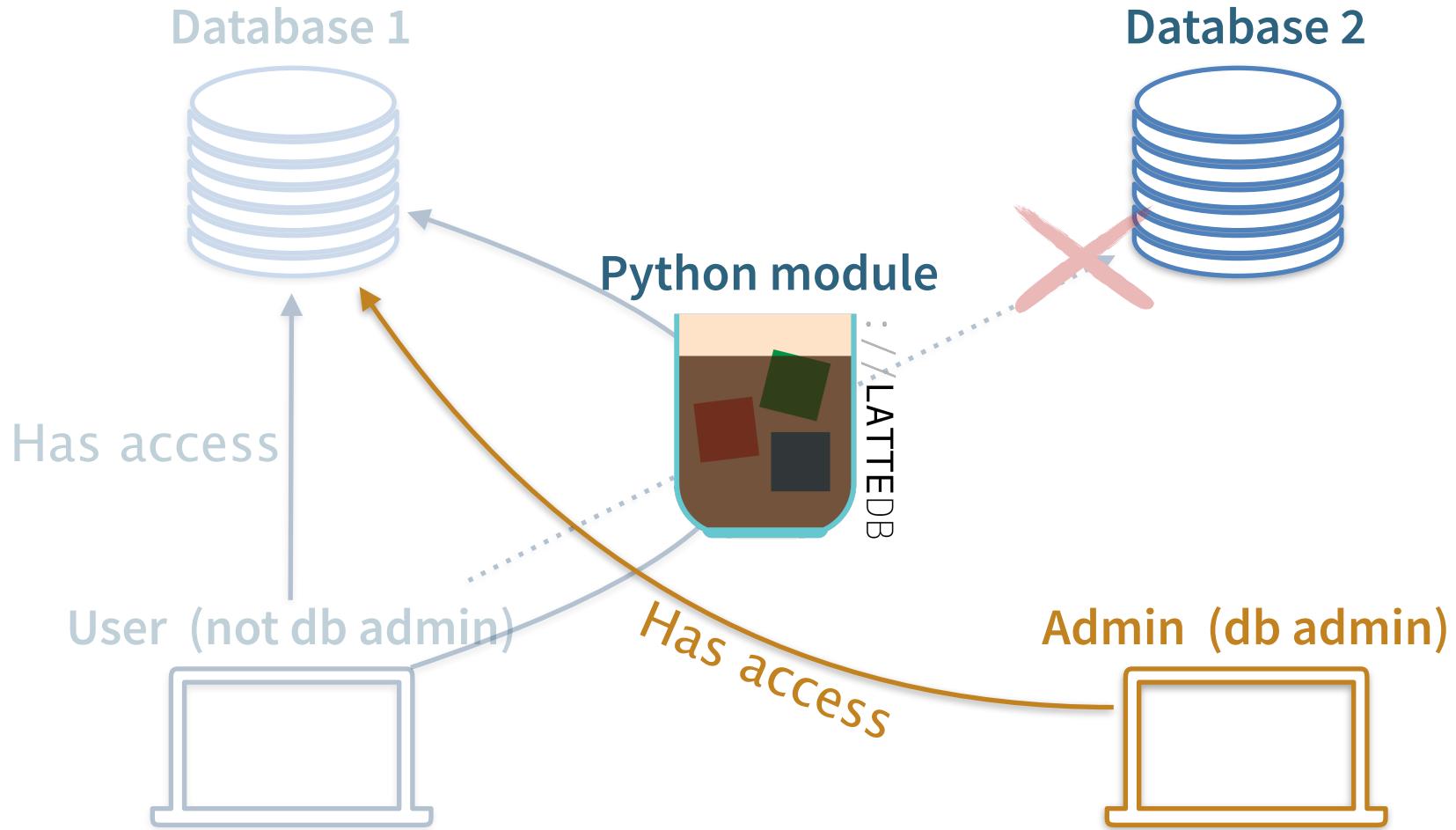
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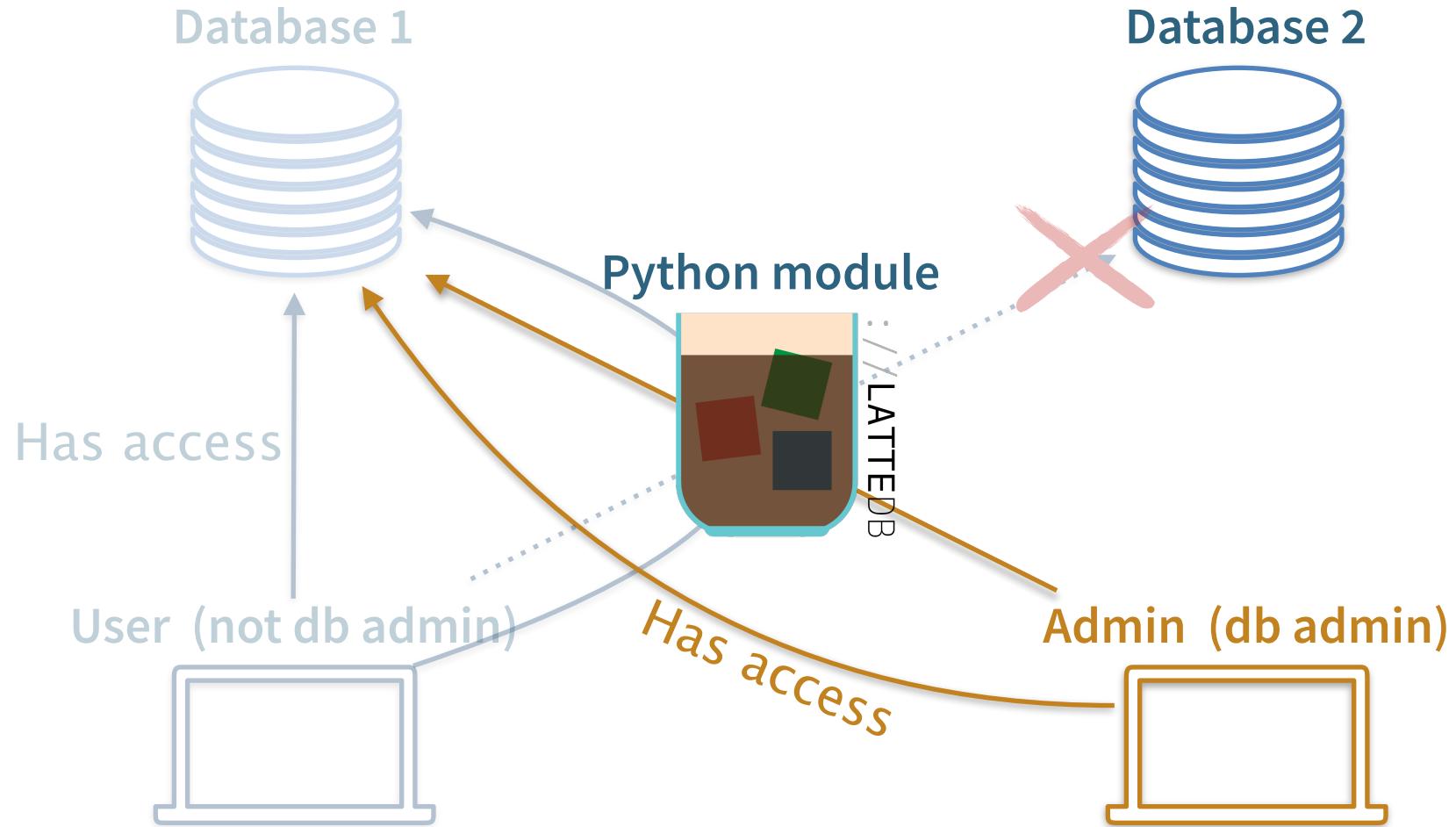
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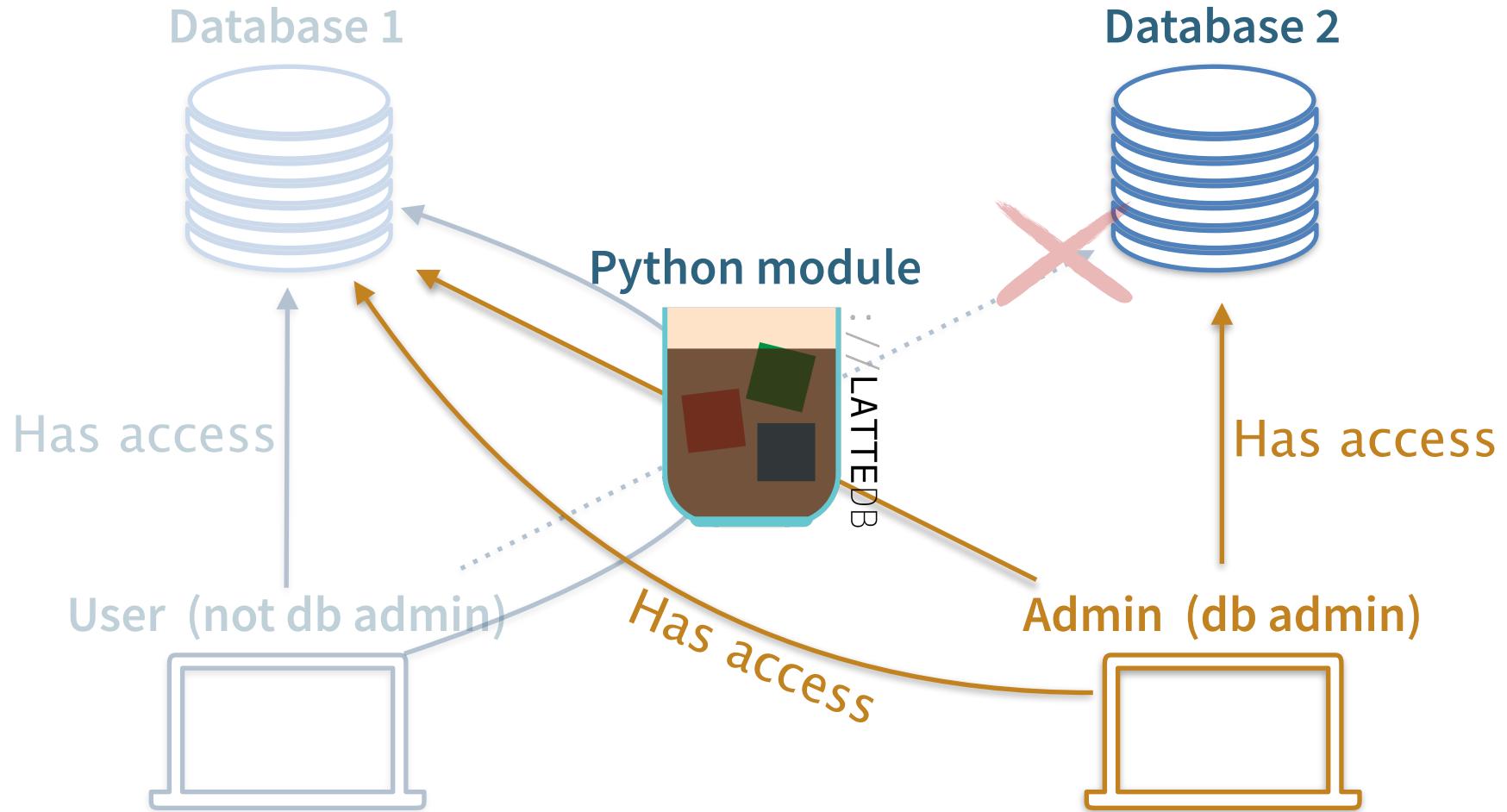
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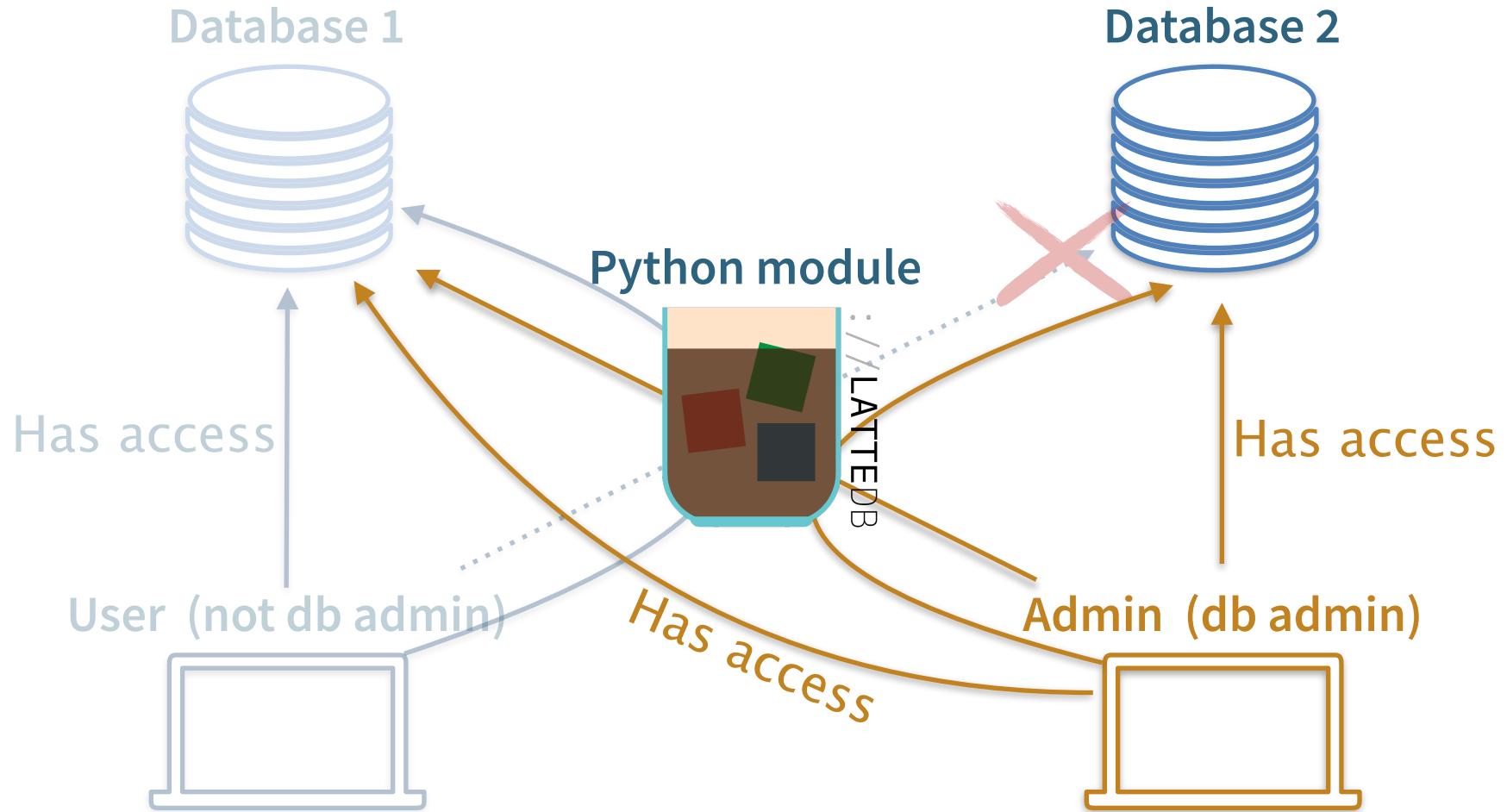
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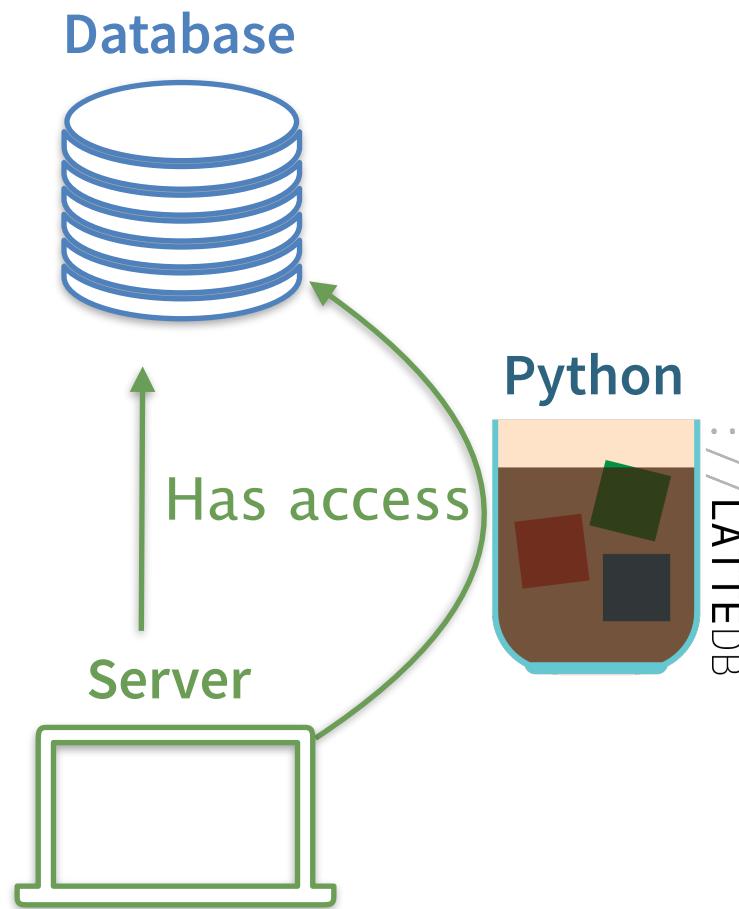
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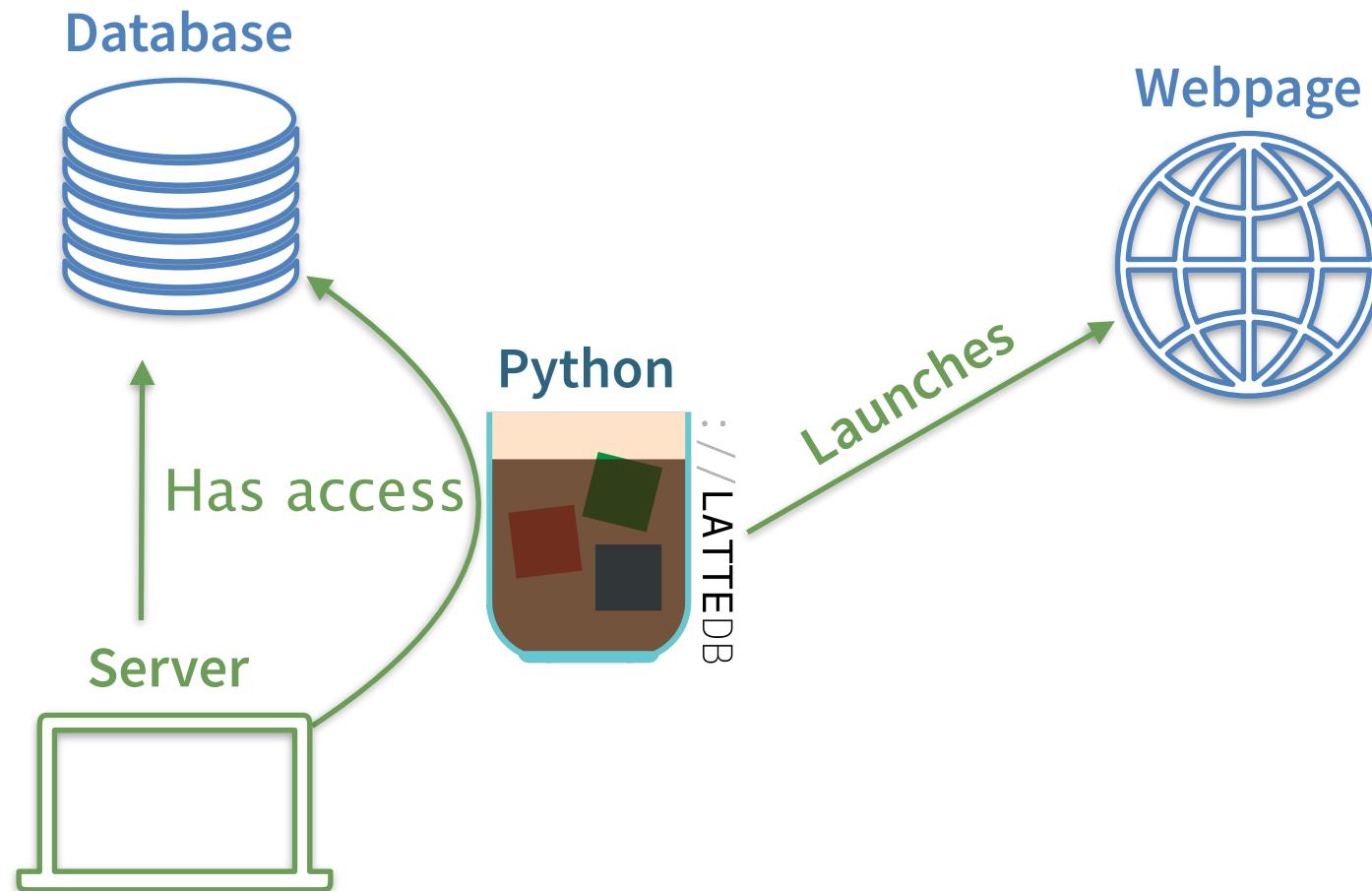
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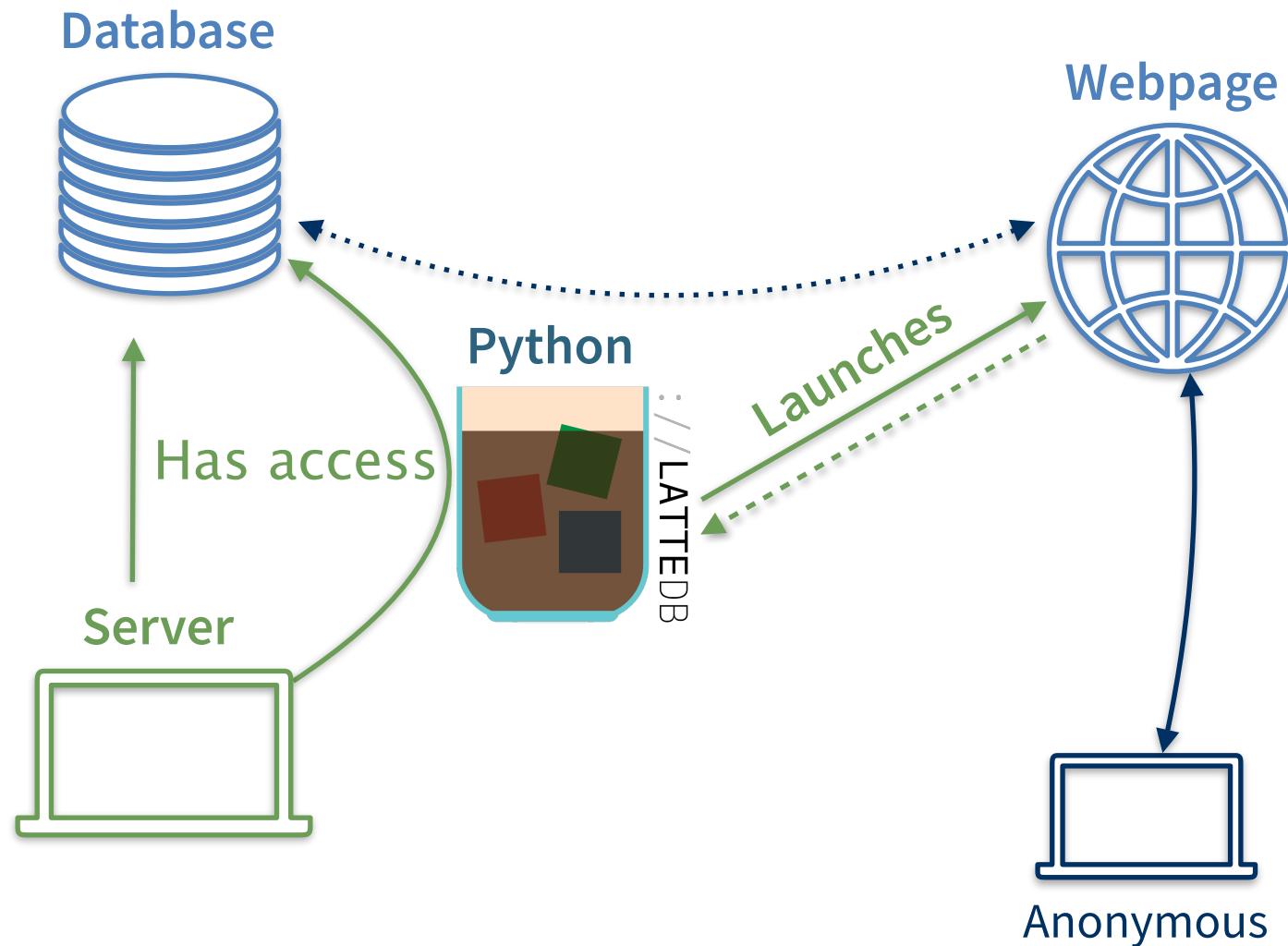
Security Layers (Webpage)



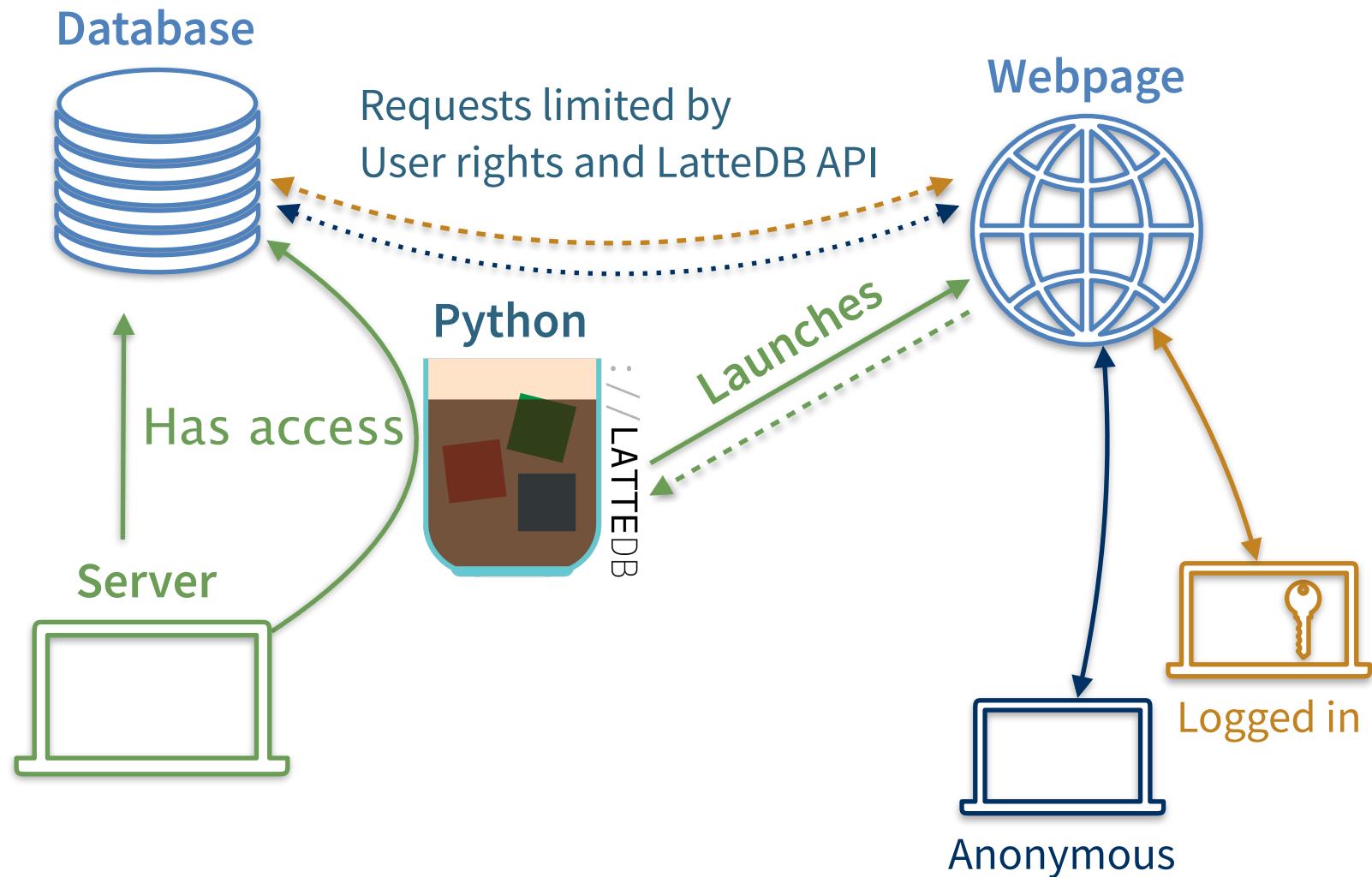
Security Layers (Webpage)



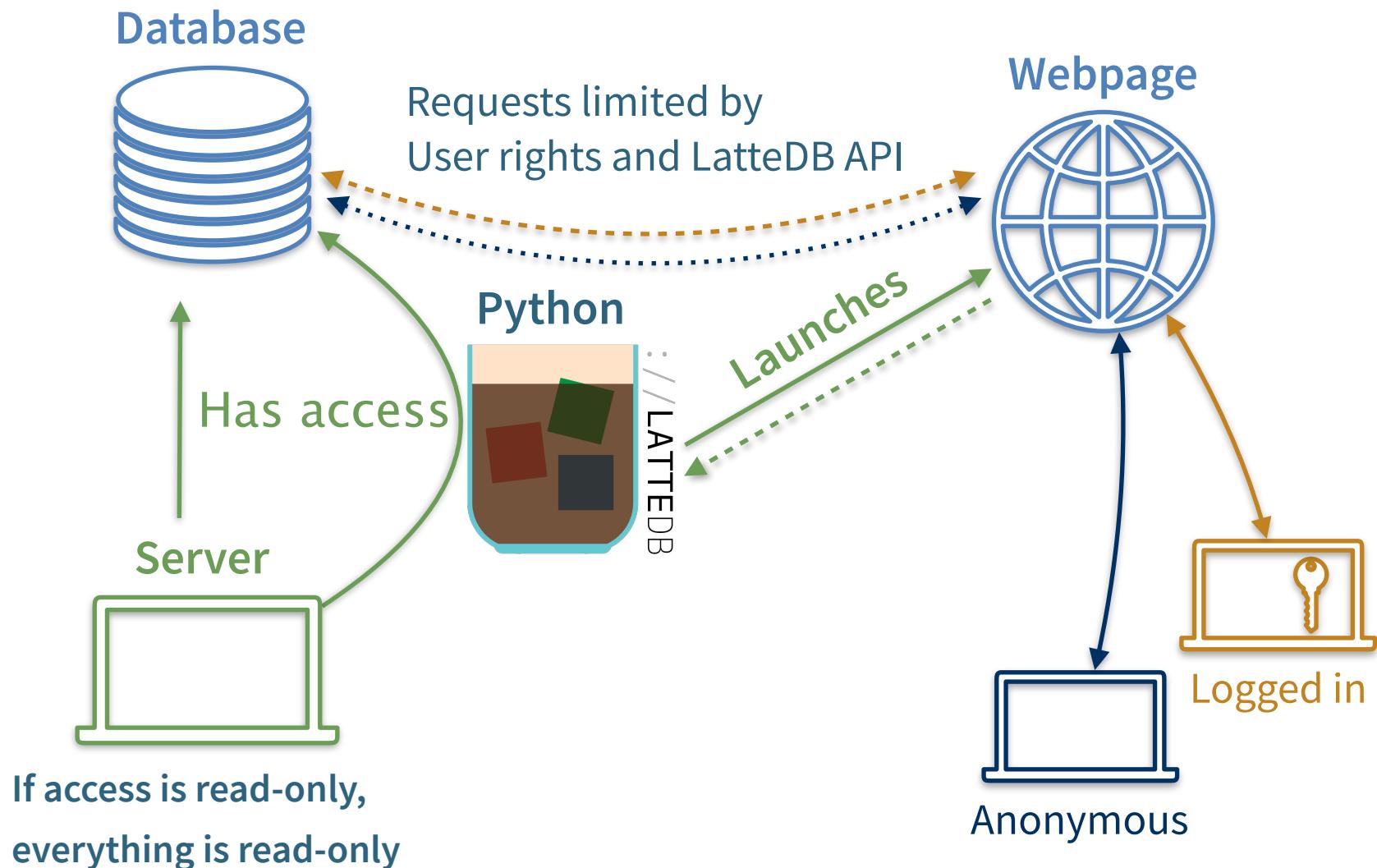
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Future

- Publish Lattice App/Tables
 - Implement consistency checks for insertions
 - Test job management production on tiny example
 - Production runs: analysis & job management
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 - Continuous Integration:
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 - Table additions

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 - Test job management production on tiny example
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 - Table additions
- **Extract & Publish Stand-Alone Mini-App**
 - Contains general framework
 - Documentation and usage guide
 - Unittests & module dock

Backup

Table Layout

