



Universiteit
Utrecht

The WeNMR Case Study

**Research Software as a Service for Demonstrating Impact, Securing
Funding, and Serving a Global Community**

Rodrigo Vargas Honorato, PhD

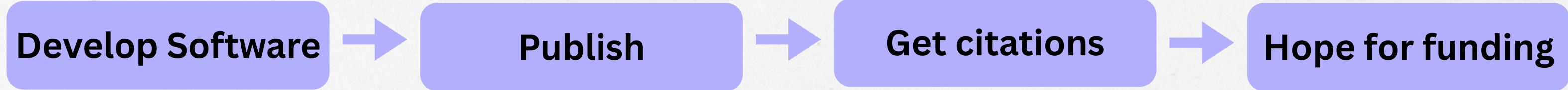
wenmr.science.uu.nl

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Overview

- 01 The Sustainability Challenge**
- 02 WeNMR A Global Research Platform in Action**
- 03 Quantifiable Impact**
- 04 From Metrics to Funding**
- 05 Building a Scalable and Sustainable Service Portal**
- 06 Research Software as a Service**

Essential Software, Invisible Impact



Research software is the backbone of modern science.

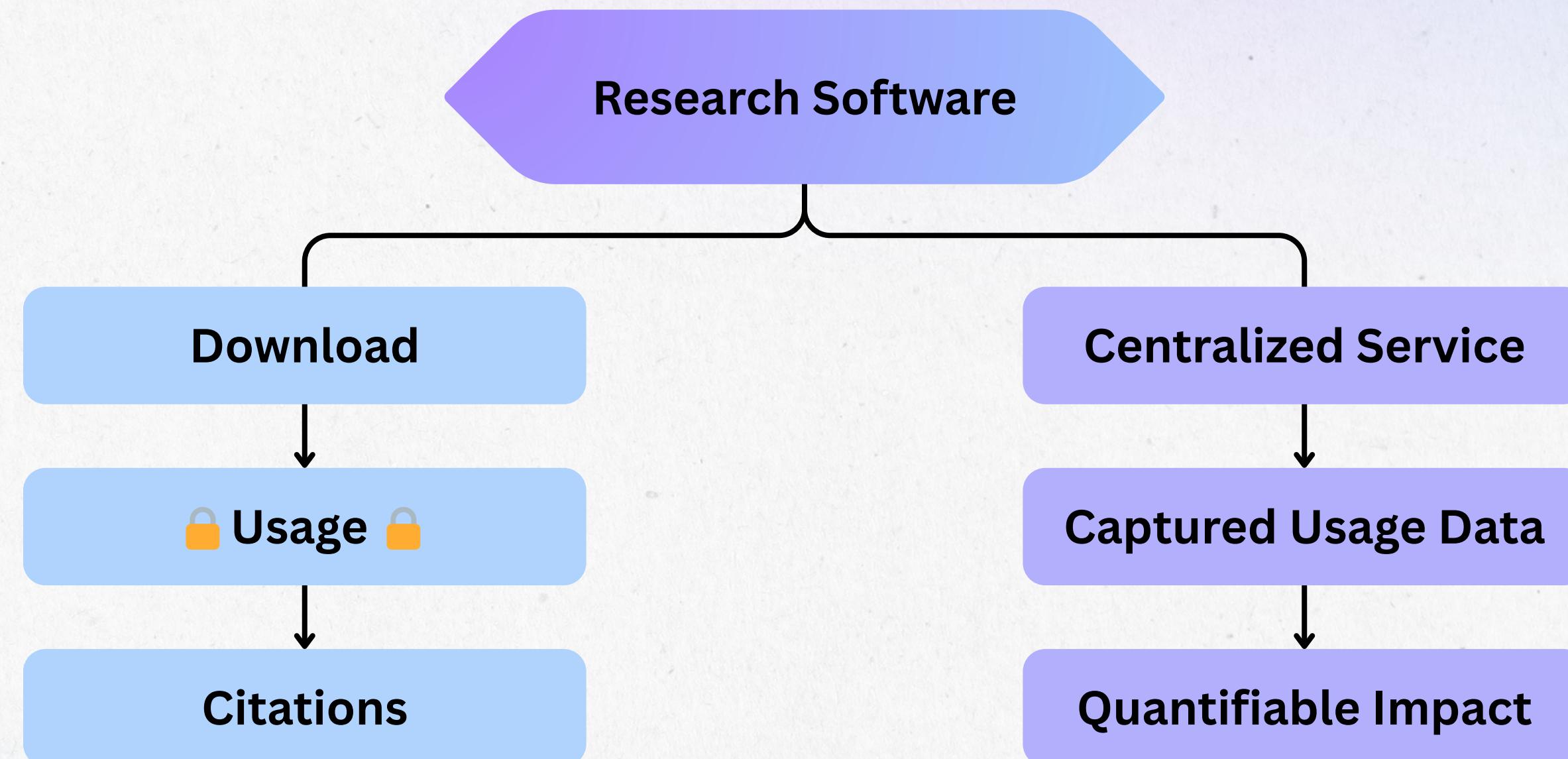
Yet, the standard metrics for success are flawed:

Downloads: Don't measure actual use.

Citations: Don't capture the full scope of use.

How do we make the invisible work of our software visible and irrefutable?

The RSaaS Model



01

Distributed Approach

Research Software is distributed to the community but the actual usage is a black box, we must use indirect measures.

02

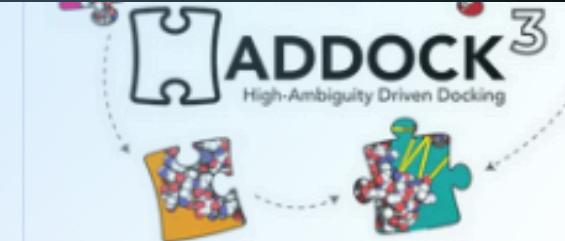
Centralized Service Approach

We provide the users with a centralized way to interact with the Research Software, so we can capture the usage data directly.



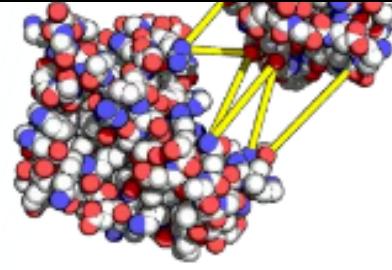
HADDOCK v2.4

HADDOCK is an integrative platform for the modeling of biomolecular complexes. It supports a large variety of input data and can deal multi-component assemblies of proteins, peptide, small molecules and nucleic acids.

[Go to service](#)

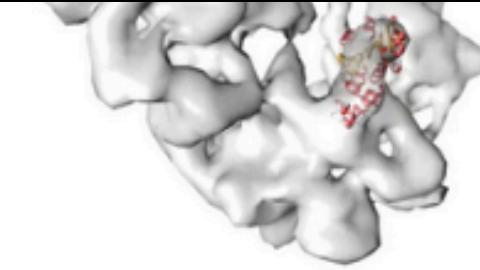
HADDOCK v3.0

We are working on a new and modern interface for HADDOCK! Soon we will make it available for everyone stay tuned!

[Team testing](#)

haddock-restraints

Generate HADDOCK compatible ambiguous restraints.

[Go to service](#)

POWERFIT

POWERFIT automatically fits atomic models into cryo-EM density maps.

[Go to service](#)

Prodigy

PRODIGY predicts the binding affinity of protein-protein and protein-small molecules complexes and also allows to classify crystallographic interfaces as biological or not.

[Go to service](#)

WeNMR: A Virtual Research Environment for Structural Biology

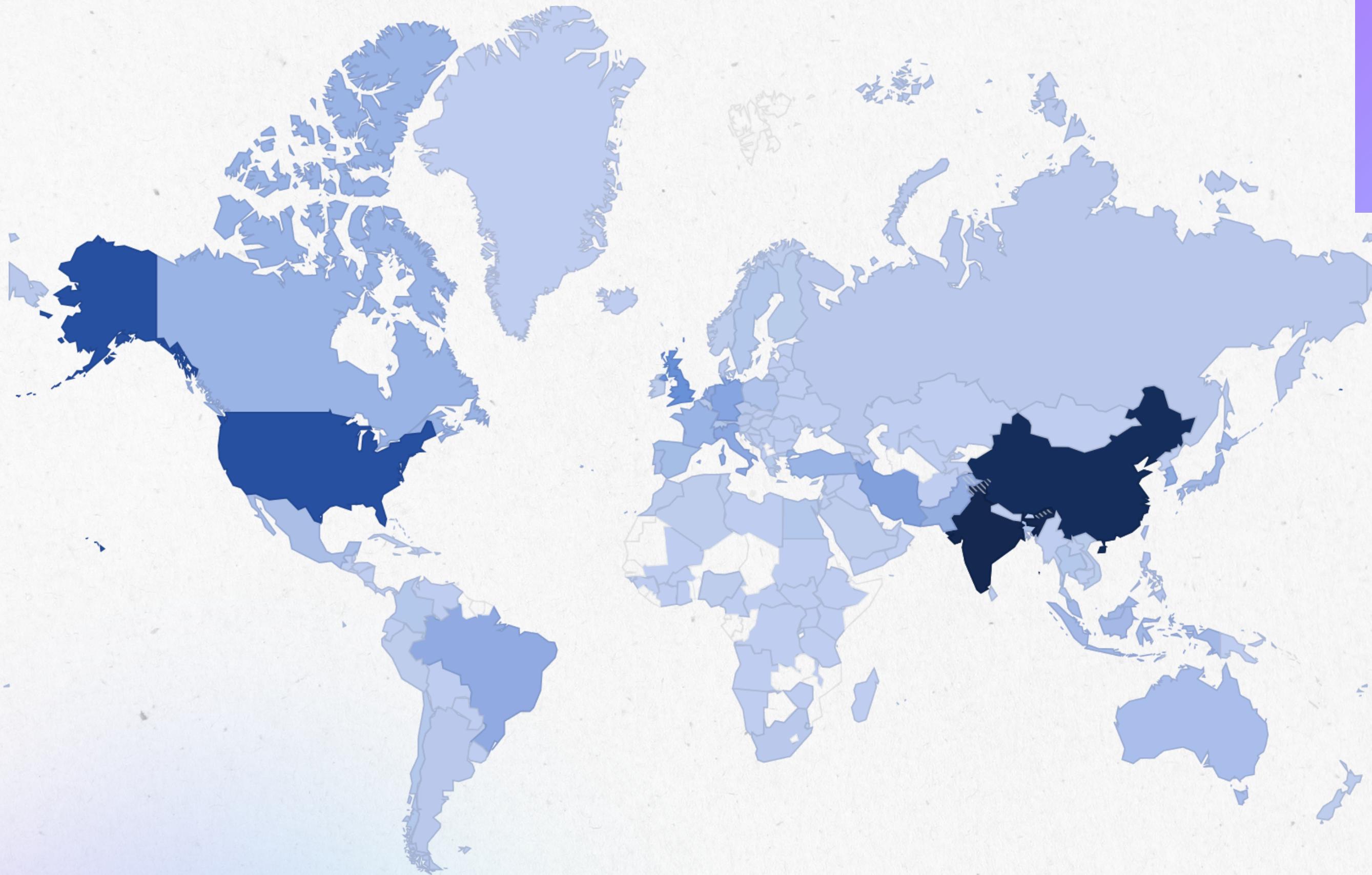
Centralized, web-accessible platform for a suite of structural biology tools.

Provides computational workflows, data management, and expert support.

Eliminates technical barriers for researchers (no installation, no local HPC access needed).

wenmr.science.uu.nl

Global Community



73.000+ Registered users
180 Countries
13 Services
1M CPU/Hours per Year

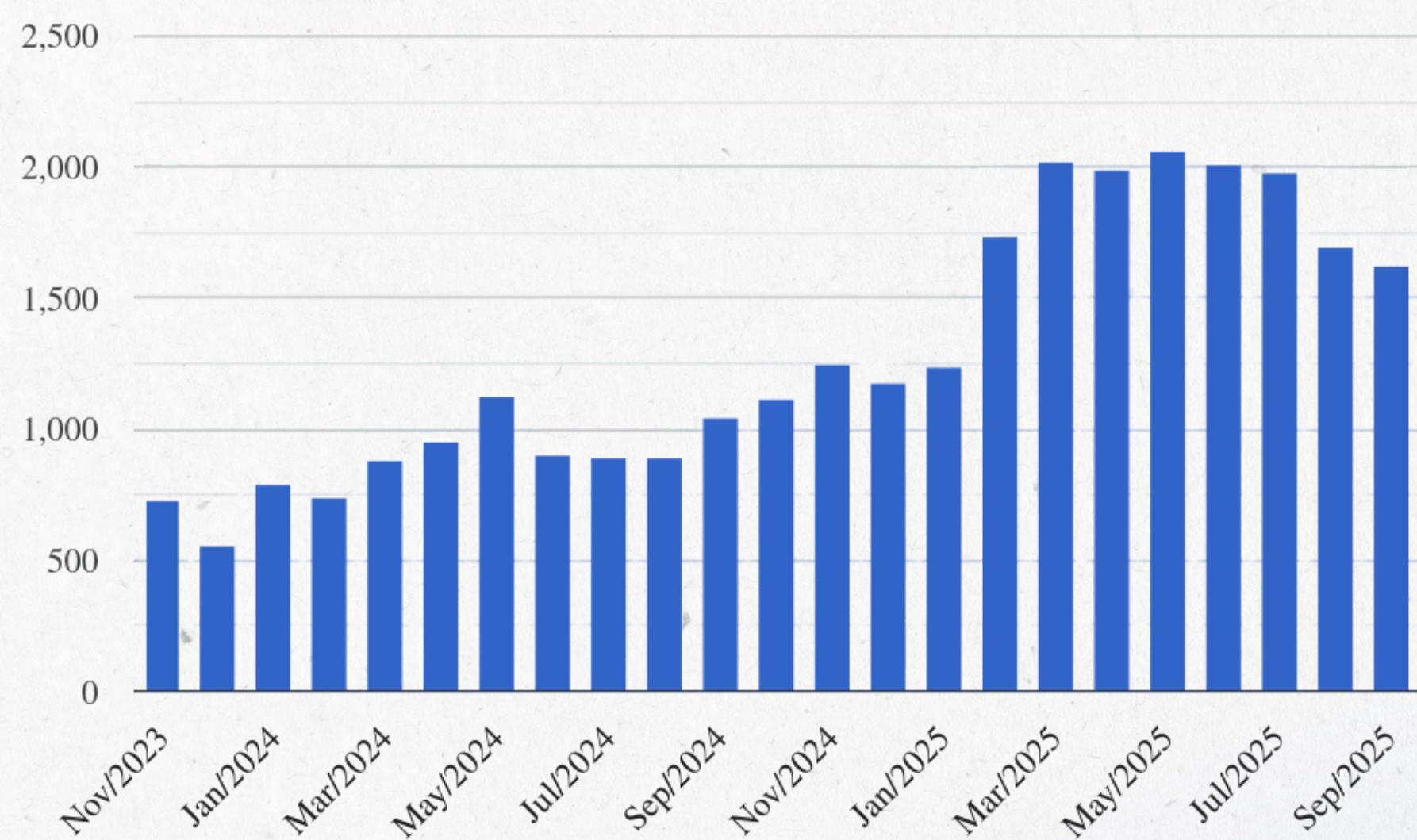
| Continent | # of Users |
|---------------|------------|
| Asia | 39548 |
| Europe | 16074 |
| North America | 11268 |
| South America | 3029 |
| Africa | 1432 |
| Oceania | 836 |

Quantifiable Impact

As a centralized service, every interaction is a data point

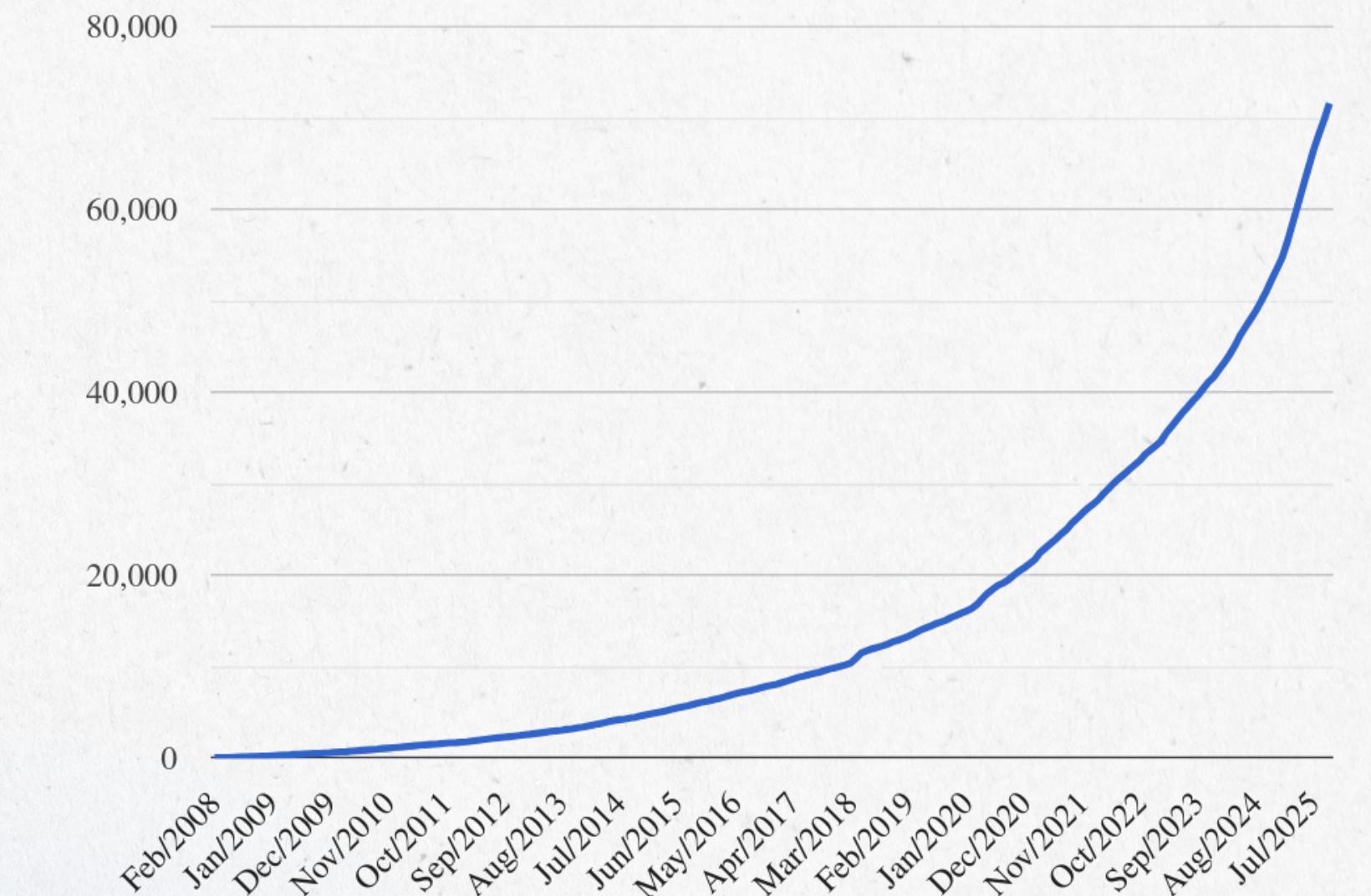
New users per month

(last 24 months)



Cumulative number of users

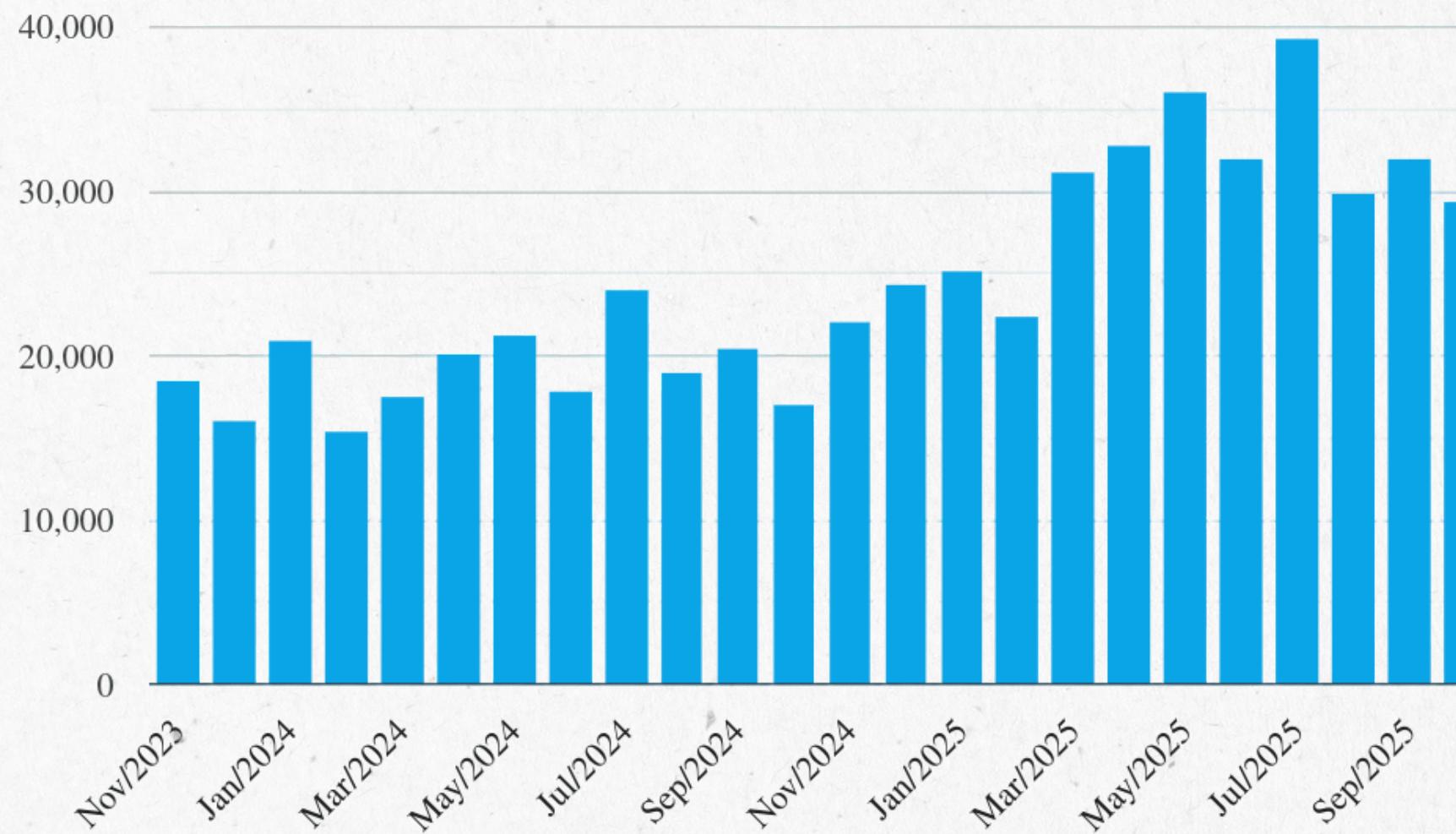
(all time)



Quantifiable Impact

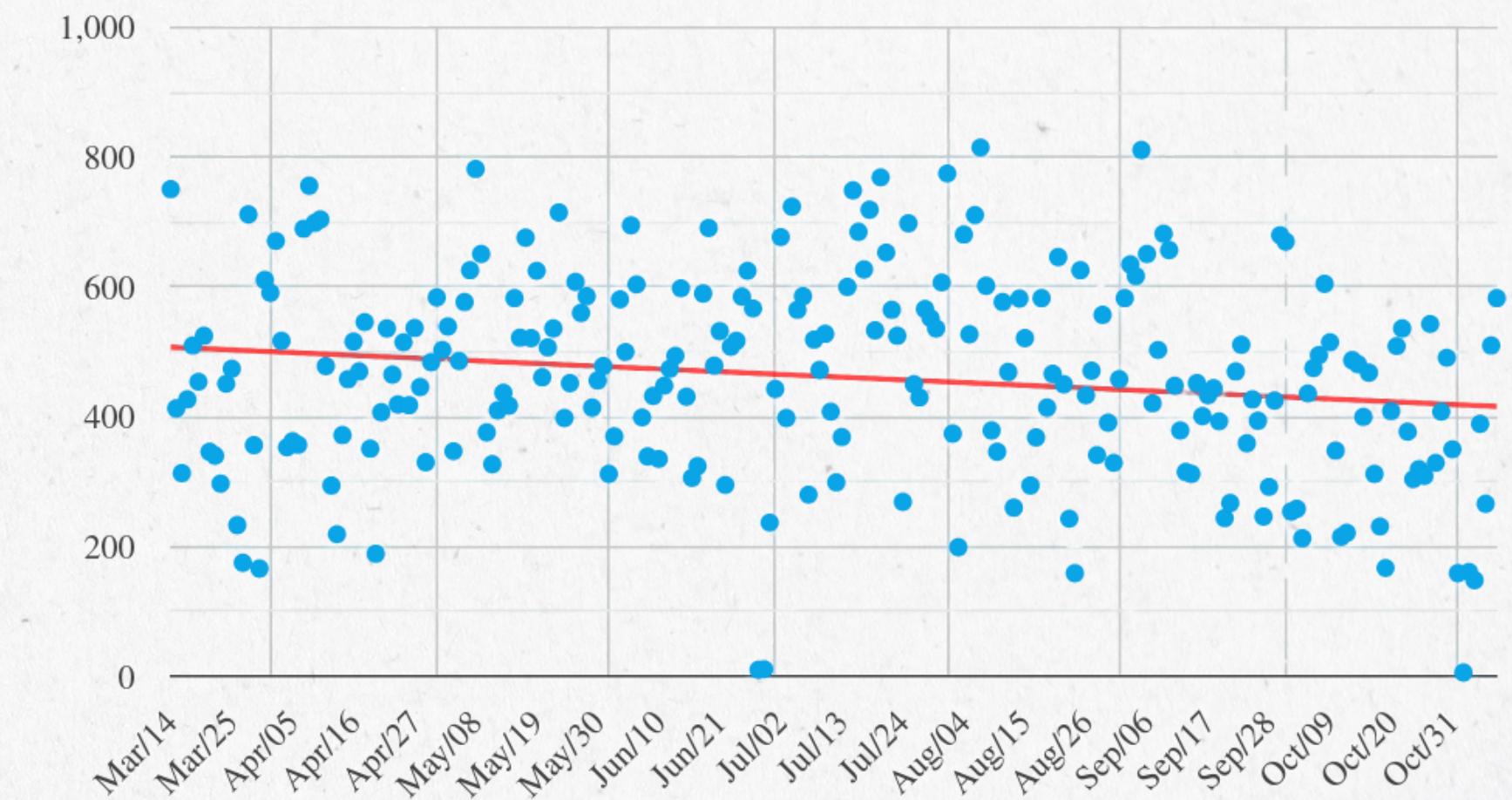
Total jobs processed

(last 24 months over all services)

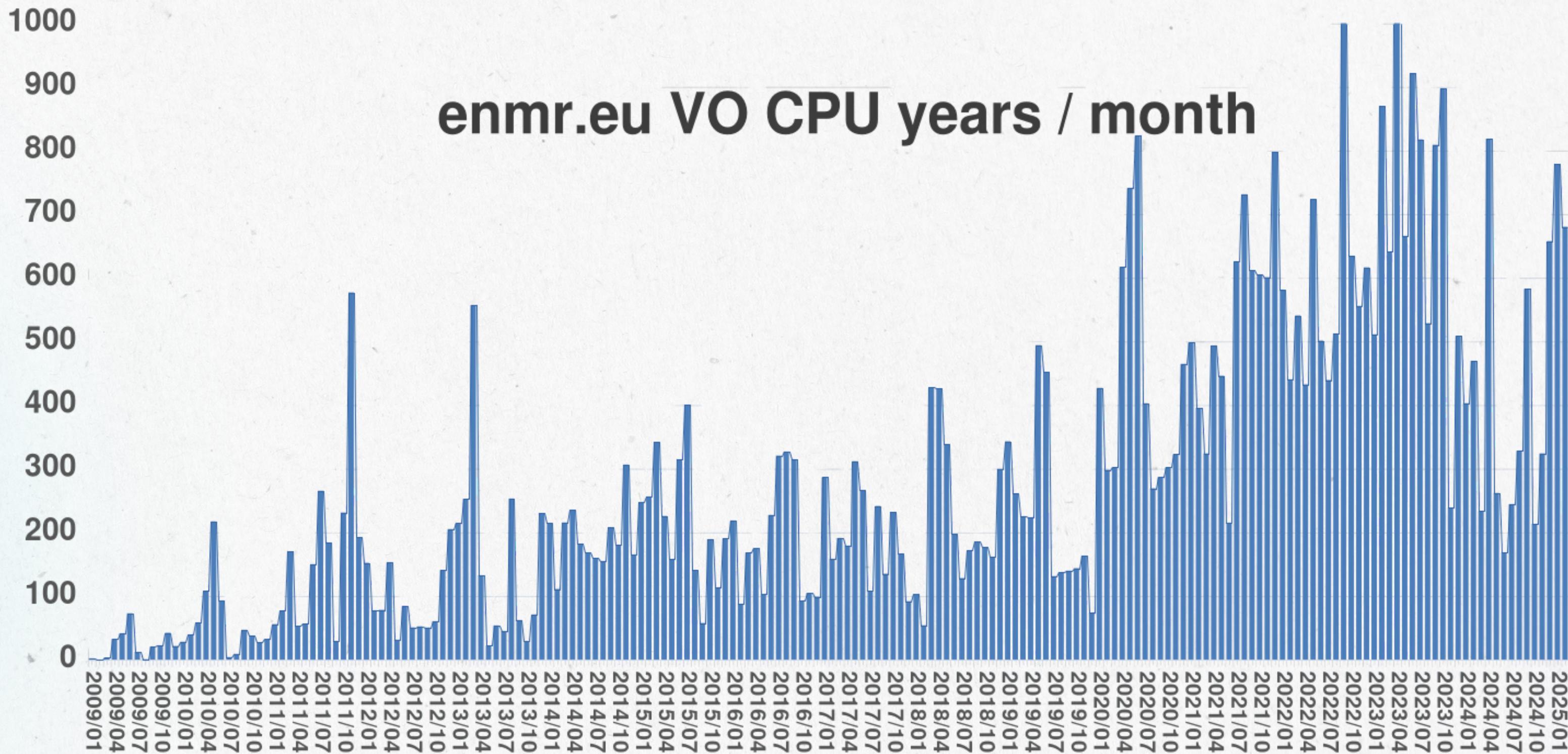


HADDOCK Jobs per day

(how many jobs were *DONE* in the past 240 days)



Quantifiable Impact

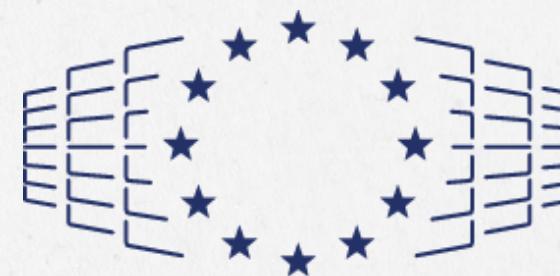


Usage data as narrative

"WeNMR is not just software. It is a critical piece of research infrastructure that directly enables 4,800 CPU-years of science annually for a global community of 72,000 researchers."

netherlands

eScience center



EuroHPC
Joint Undertaking



SURF SARA

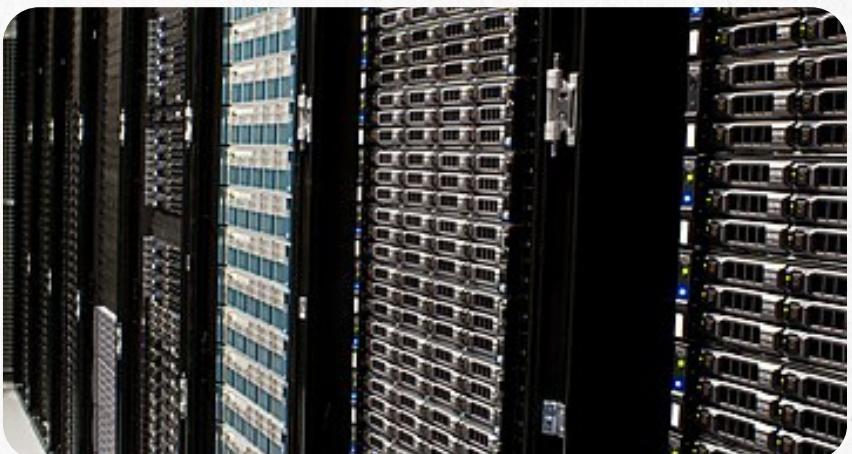


Horizon 2020
Programme

Sustained Investment

Over the past **20 years** the WeNMR portal has been a key asset in the acquisition of several grants to sustain its development and operation.

RSaaS model provides accountability and demonstrable impact to funding agencies.



Service Operation

EC HORIZON-INFRA-2024-EOSC-01-05 - EOSC Data Commons.
EC H2020-EINFRAEOSC-07 - EOSC-ACE
EC H2020-EINFRA-12-2017 - EOSC-Hub.
EC H2020-EINFRA-9-2015 - West-Life
EC H2020-EINFRA-2014-2 - INDIGO-DataCloud
EC H2020-EINFRA-2015 - EGI-Engage
NWO-ENW 2020
NWO-NCF - BG-031-11
NWO computing 2009 - e-NMR
EC 7th Framework Programme 2007/2010



Software Development

EOS NLeSC 2024
NWO-ENW M1 grant 2023
EC HORIZON-EUROHPC-JU-2021-COE-01-02
eTEC NLeSC 2021
NWO-ENW PPS 2019
EC H2020-EINFRAEDU-2018-1
SURFsara ML-HPC 2018
NWO-CW TOP-PUNT 2015
EC H2020-EINFRA-5-2015
NLeSC Accel Sci Discovery 2016
NWO-CW ECHO 2011
NWO VICI grant 2006
NWO Jonge Chemici 2001

~9.5M € + ~10.5M CPU/H

Powered by EOSC/EGI

WeNMR Portal

EOSC/EGI

HTC/HPC & Cloud

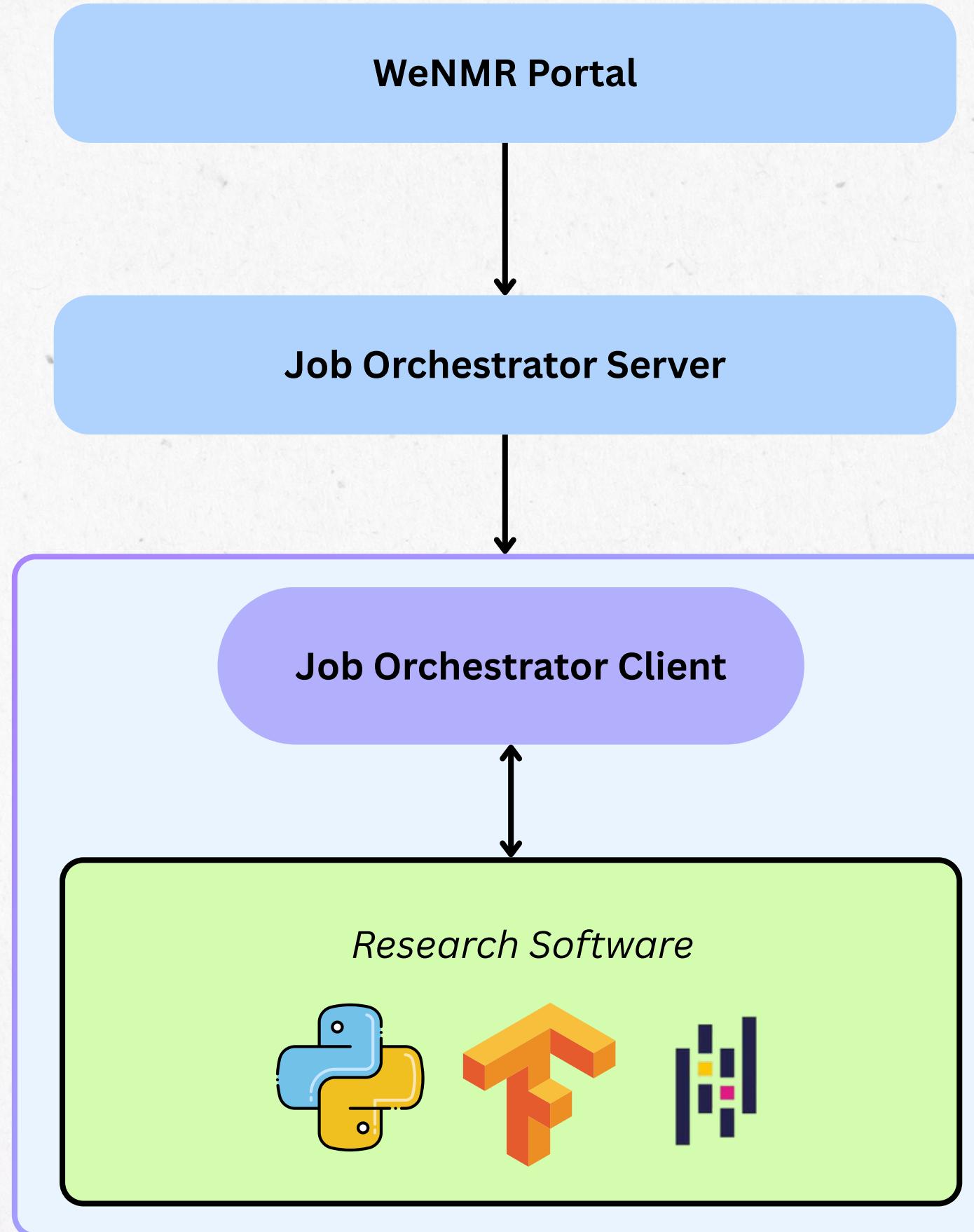
WeNMR is built on top of European e-Infrastructures

Built for scalability

Integrated with EOSC/EGI Grid via DIRAC interware

Users get access seamless (and free) to massive computing resources

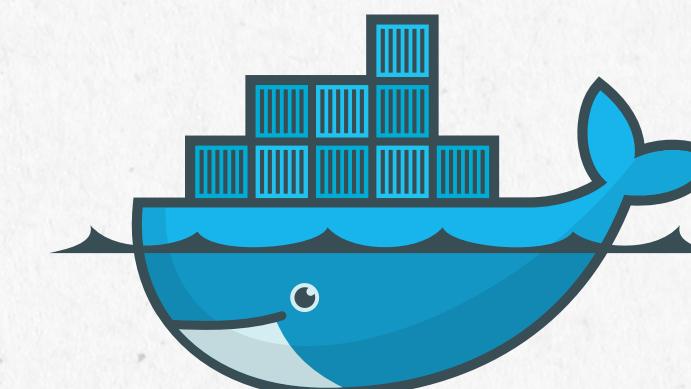




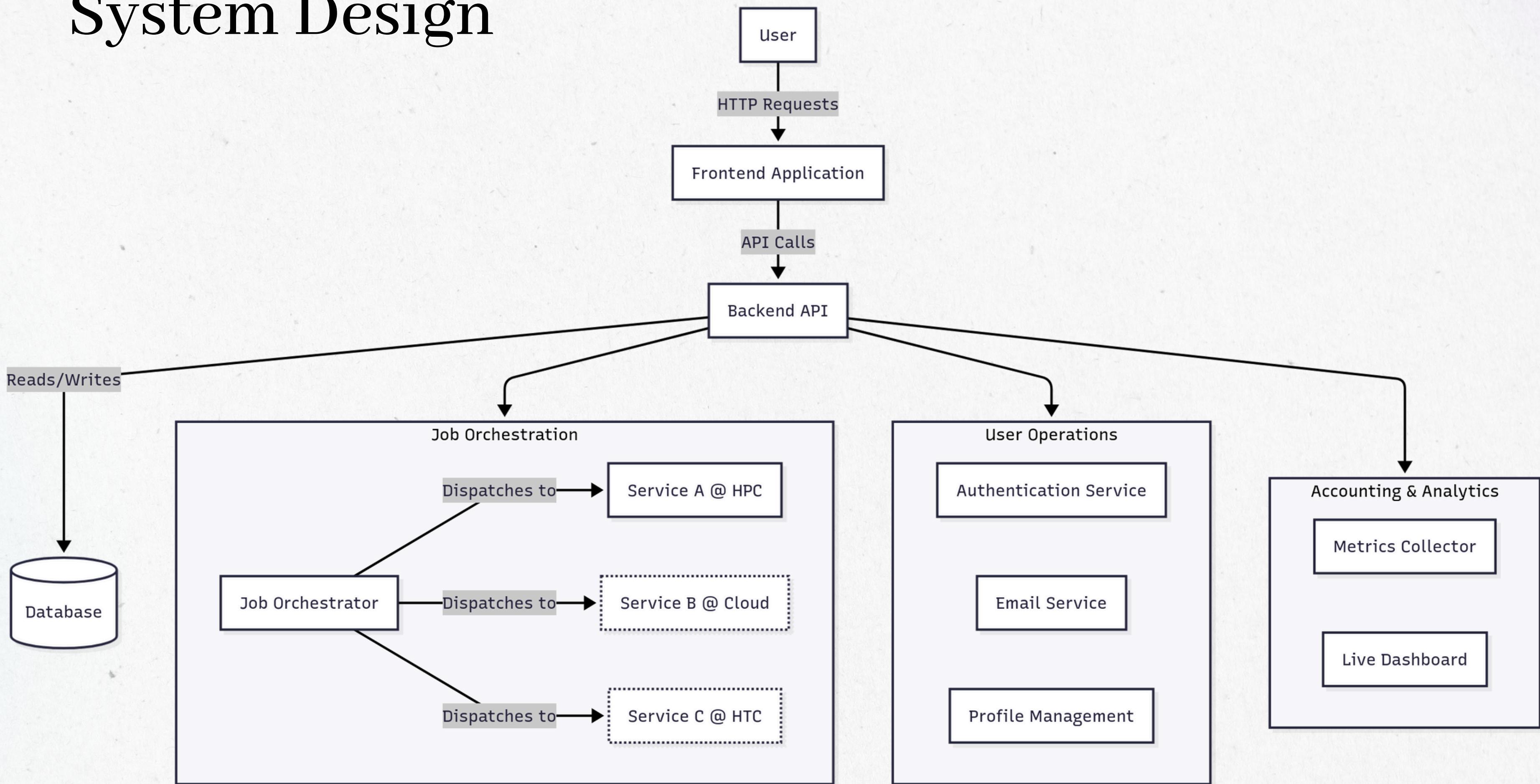
Containerized architecture

Research Software can be packaged into containers

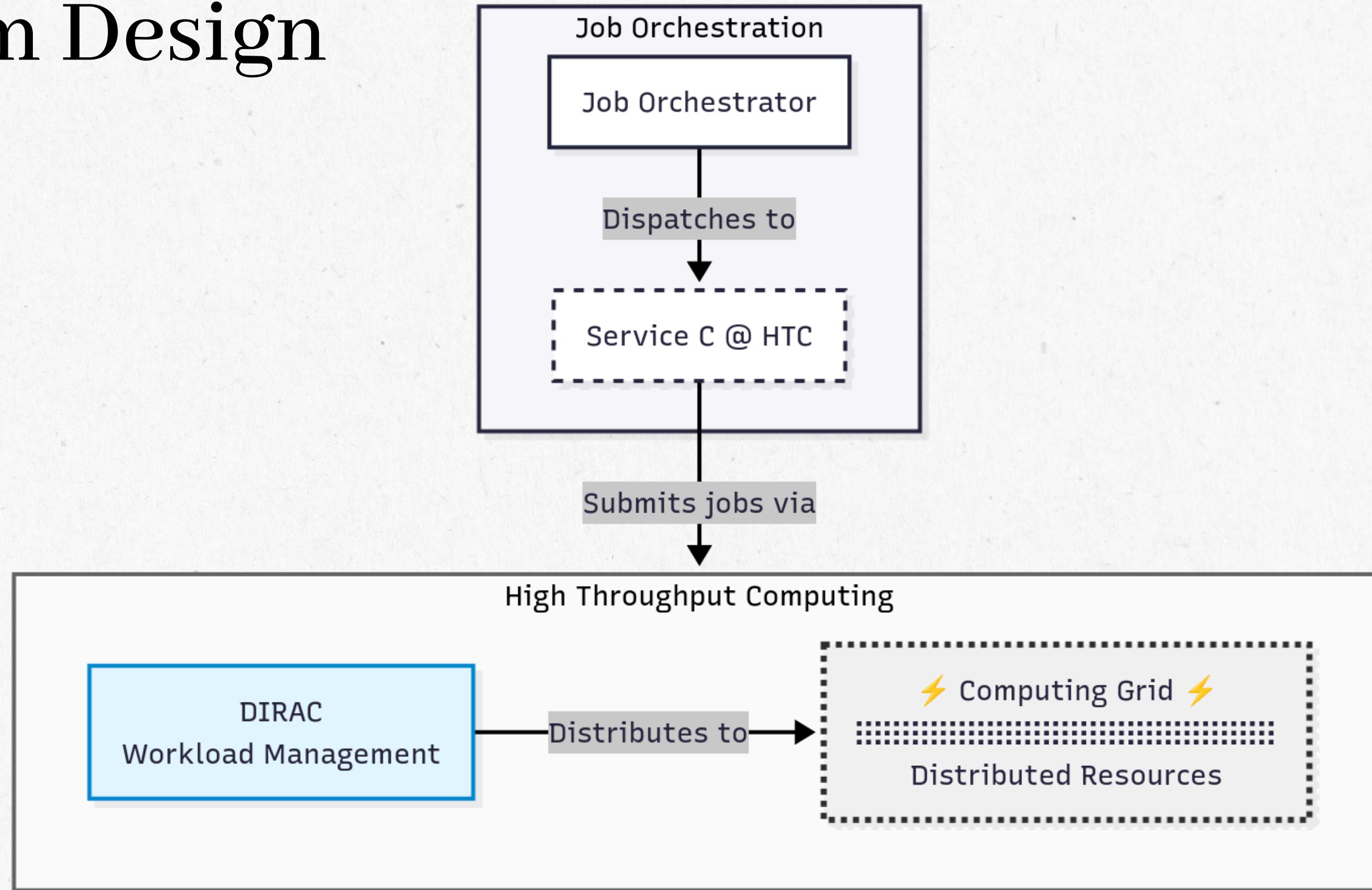
Reduce complexity and normalize interfaces



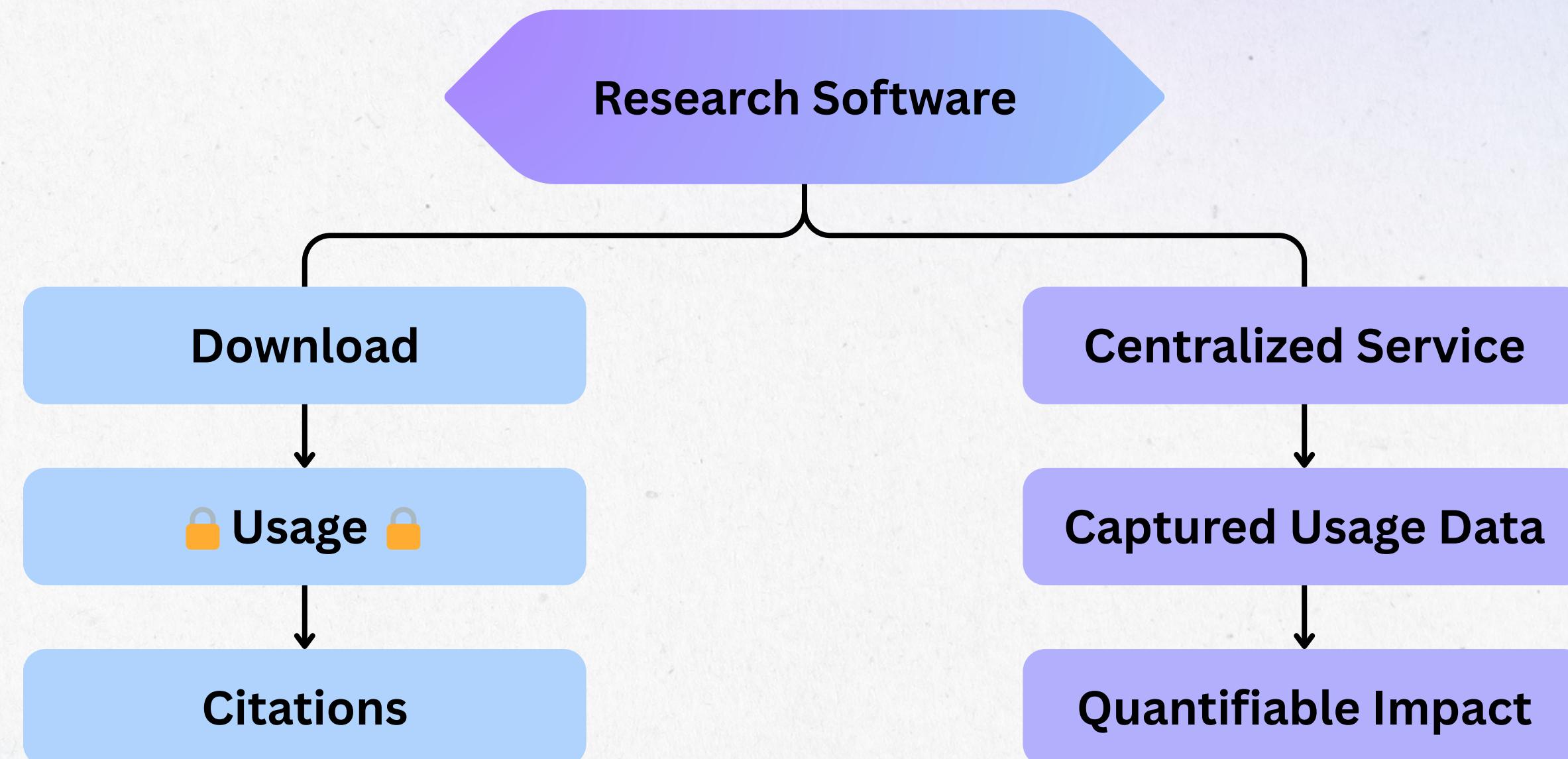
System Design



System Design



The RSaaS Model



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Research Software as A Service

01

Move to a Service

Move beyond code distribution to a managed, centralized platform. Invest in platforms, not only projects.

02

Quantify Everything

Capture real-time usage data, compute jobs, active users, CPU-years - get direct evidence of your software's scientific utility.

03

Translate Data into Strategy

Your observable metrics demonstrate indispensability, clearly state community adoption and scientific throughput.

04

Build on Scalable foundations

Use existing e-Infrastructures (EOSC/EGI) and modern DevOps practices. Design for interoperability to ensure long-term viability.



Universiteit
Utrecht



Bonvin Lab
computational structural biology



Thank you



r.vargashonorato@uu.nl



rvhonorato.me

