Using Elasticsearch to **store**, **integrate** and **mine** diverse biological data

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CTTV Core Team - EBI

goo.gl/hmTI6j

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Centre for Therapeutic Target Validation

CTTV

CTTV

- Private-Public Initiative
  - EBI - Sanger - GSK
- Aims to provide evidence on the biological validity of therapeutic targets using genome-scale experiments and analysis
- CTTV Core
  - The Core Team is in charge of organise and integrate the available data and serve it through a Web App and a REST API
  - Our software stack should be easy to replicate in internal mirrors by partner organisations

Overview

- Data
- Data Integration
- Data Mining
- Architecture

Data

Core Data

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Data Sources

- ChEMBL
- COSMIC
- Europe PMC
- EVA
- Expression Atlas
- GWAs Catalog
- Phenodigm
- Uniprot
- ... and eventually more
  in private deployments

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Data Types

- Genetic association
- Somatic mutation
- RNA expression
- Known drugs
- Animal models
- Text mining

Public Database Data

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- Target related generic data
- Disease related data (EFO Ontology)
- Evidence Ontology
- Reactome pathways
- Protein and RNA expression data
- more to come...

CTTV Building Blocks

TARGET

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Relate a Target and a Disease through an Evidence

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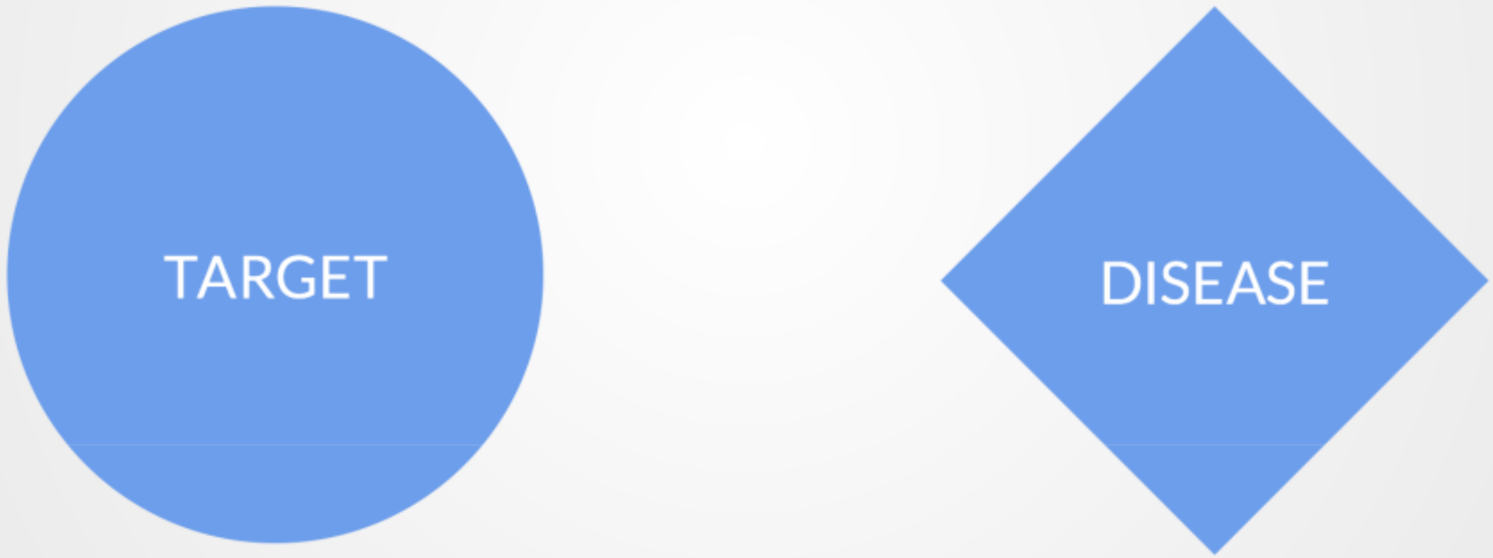

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Building blocks in real life

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JSON objects with a flexible format: Evidence String

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JSON objects with a flexible format: Evidence String


```
{
    "sourceID": "expression_atlas",
    "type": "rna_expression",
    "target": {
        "id": [
            "http://identifiers.org/ensembl/ENSG00000112984"
        ],
...
    },
    "disease": {
        "id": [
            "http://www.ebi.ac.uk/efo/EFO_0002917"
        ],
...
    },
    "evidence": {
        "unique_experiment_reference": "STUDYID_E-GEOD-14001",
        "resource_score": {
                "value": 0.0168,
                "type":"pvalue"
        },
        "evidence_codes": [
            "http://purl.obolibrary.org/obo/ECO_0000356"
        ],
        "log2_fold_change": {
```

4.2 Millions Evidence Strings

Storing Evidence Strings in Elasticsearch

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PUT JSON into ES

EASY. Just be sure to use a document type per datasource to avoid automatic mapping clashes

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Document count per source range from 20K to 3.3M

Best configuration with a separate index for text mining

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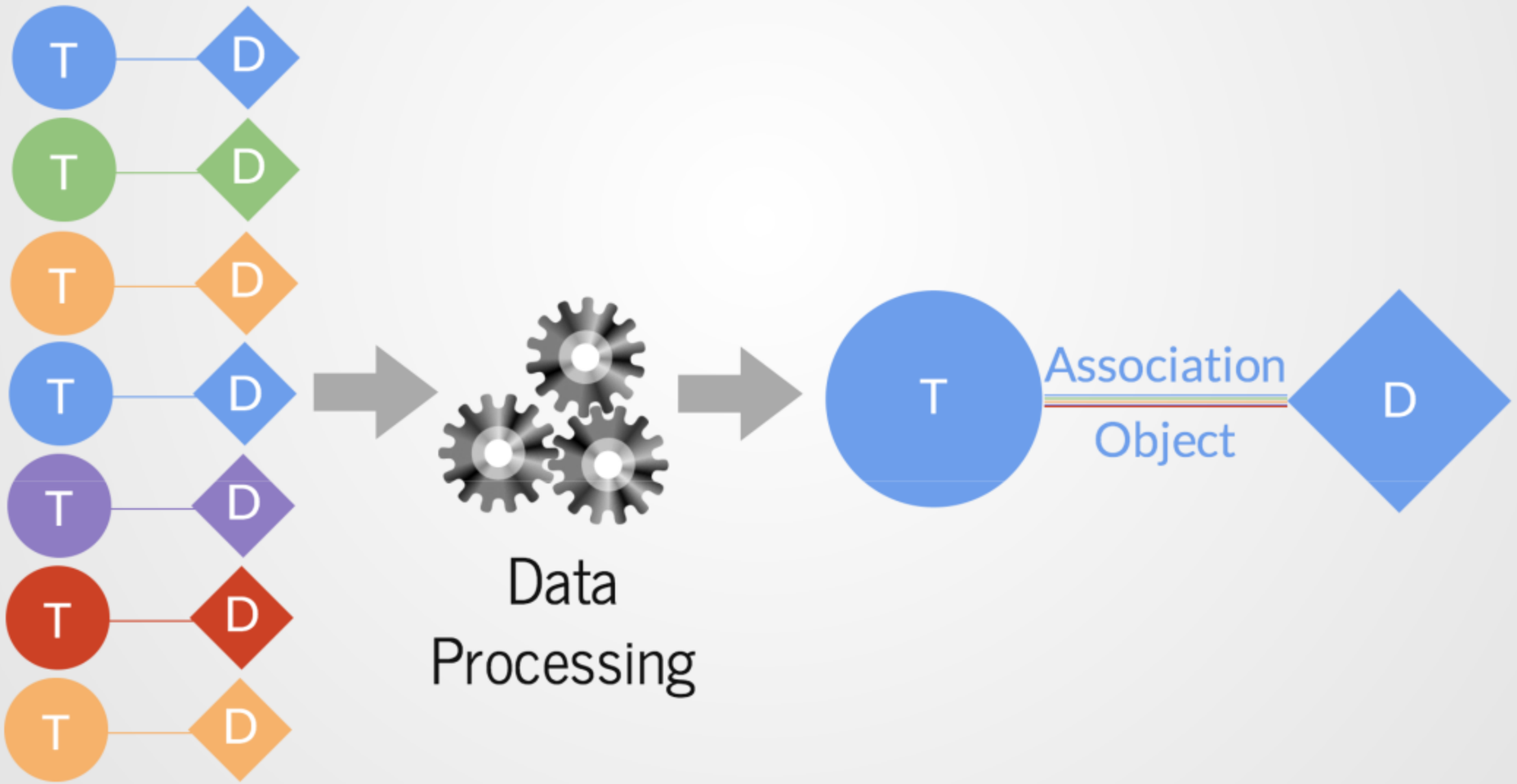
Routing

Routing by target ID distribute nicely the data and
improves filter by target query performances

Data Integration

From single evidence to target-disease association



Data Processing

Strategy #1: compute in Python-based REST API

- Retrieve all relevant evidence strings from ES
- Process them in the api
- Return computed object as JSON

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PROS

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CONS

- Very slow to retrieve a big number of evidence strings trough the network
- Python is not the fastest language out there
- Heaviest query took 20 min to run!!

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Strategy #2: compute with ES scripted metric aggregation

- Compute heavy processing steps in ES
- Process results the api
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CONS

- Tricky to code and debug
- Heavy load in ES cluster as it requires lots of CPU
- Cannot compute aggregations

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- Precompute JSON Object in a Python-based pipeline
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CONS

- Not able to tune computation parameters in the live system

2.1 Millions Association Objects

Enabling Full Text Search

- Map Association objects to full text search entities
  - Targets
  - Diseases
  - more to come (SNPs, Publications, Drugs, etc...)
- 70K search entities so far (Ensembl Gene Ids + EFO)

Data Processing
Computing Pipeline

Data Processing
Computing Pipeline

Postgres 9.4

CTTV Computing Pipeline

Multi step

Input validation

Evidence String Processing

Association Object Precomputing

Search Object Precomputation

Generic Data Processing

Parallel Processing

Elasticsearch
1.7.2

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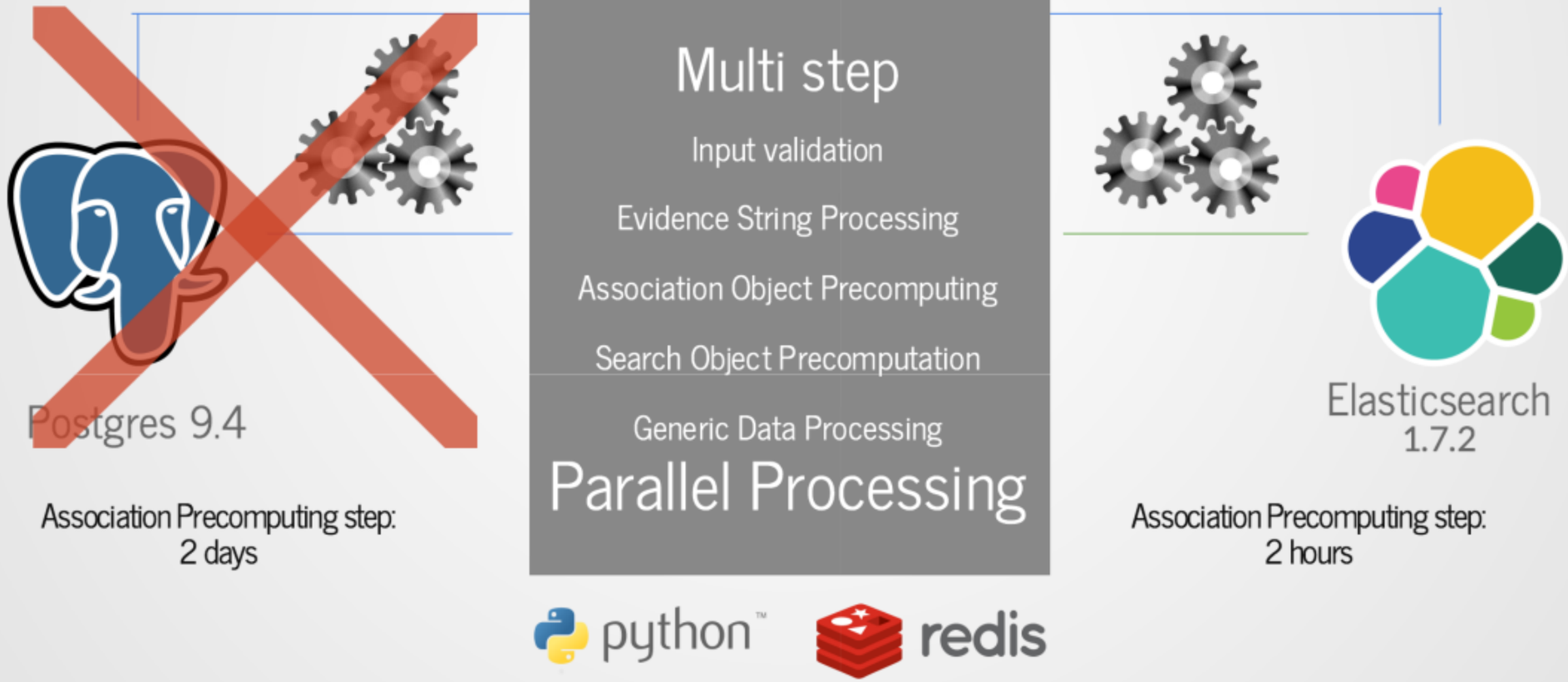
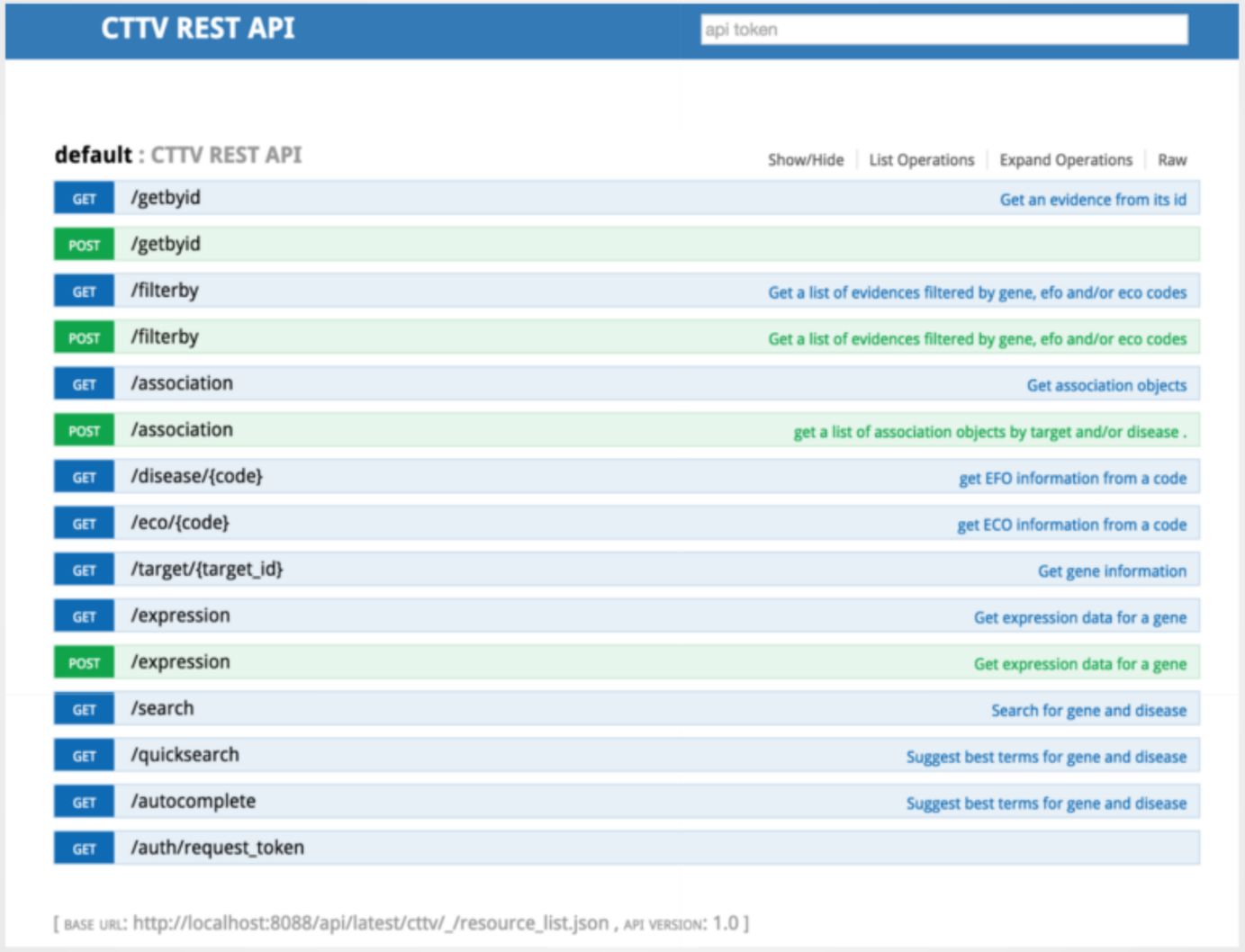


Mining the Data

CTTV REST API



Not public yet (coming soon...)

REST API Implementation

Enable to search for target and disease by full text search
(more options coming)

Most methods are thin wrappers around elasticsearch filters

Returns aggregations for associations to enable faceted search

Auth built in

Full Text Search


⚠WARNING⚠
Demo Time

CTTV Web APP

www.targetvalidation.org

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- Disambiguate between different document types
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    - systemic lupus erythematosus (what they were actually looking for)

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- Track user behaviour?

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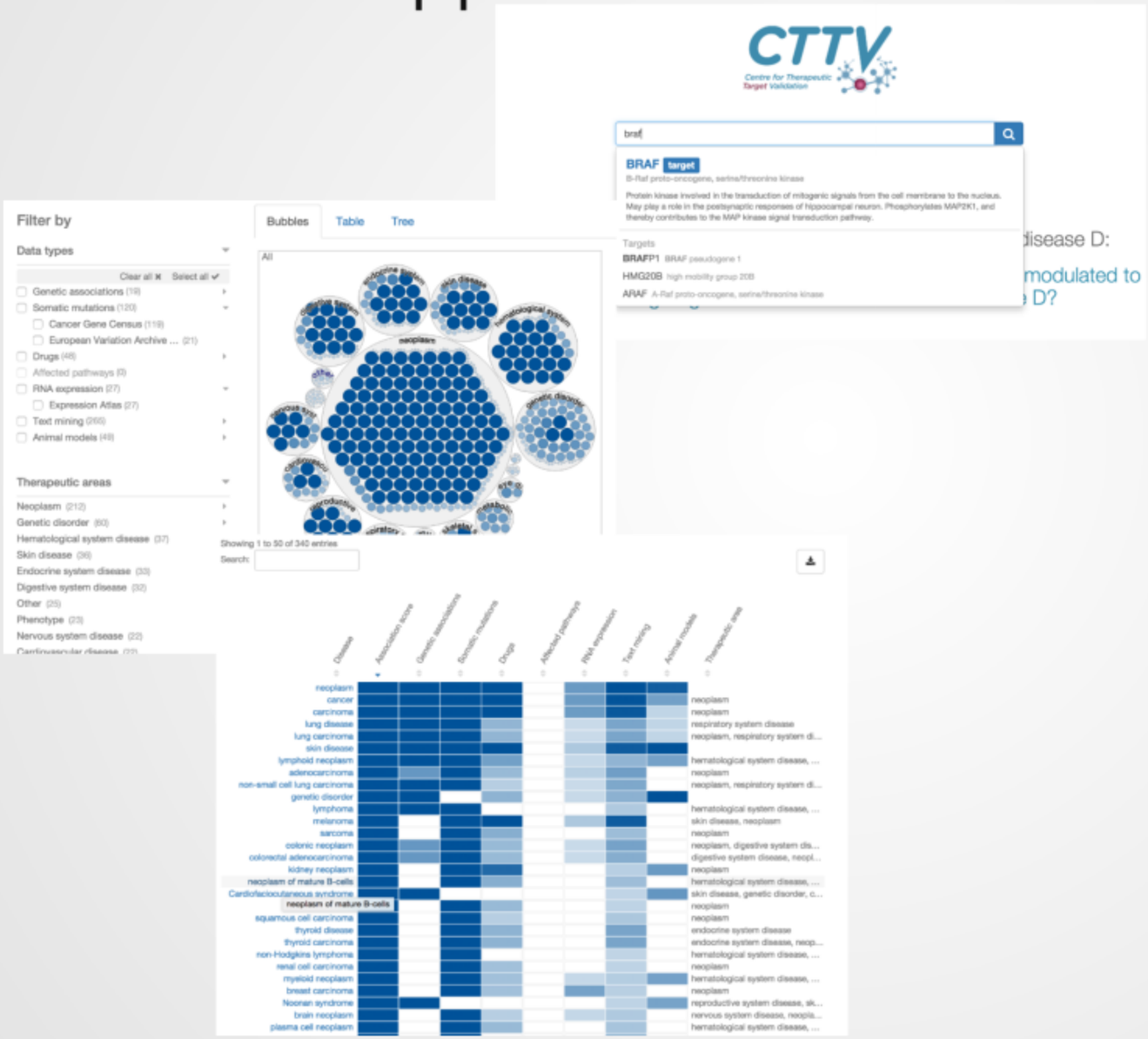

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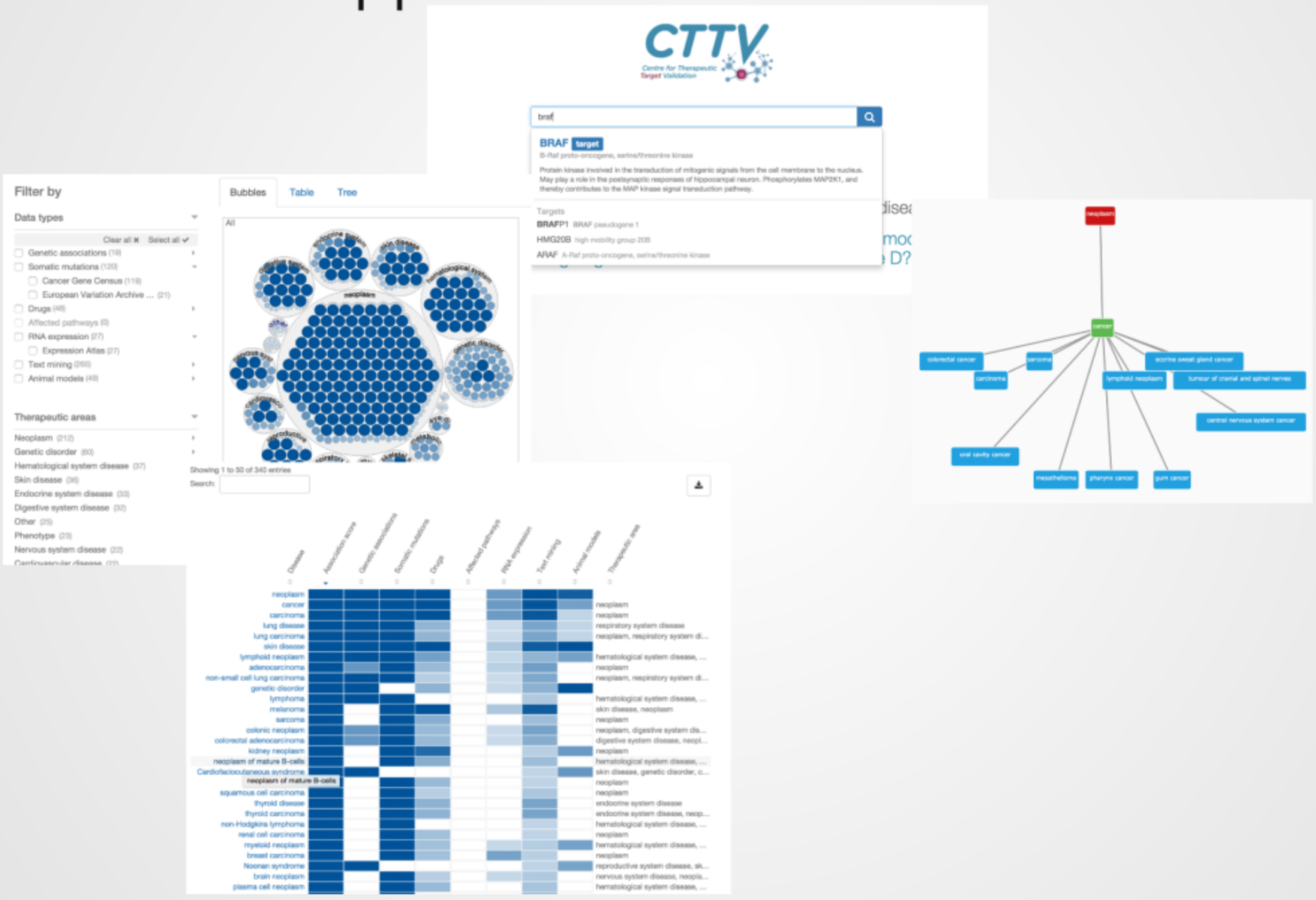

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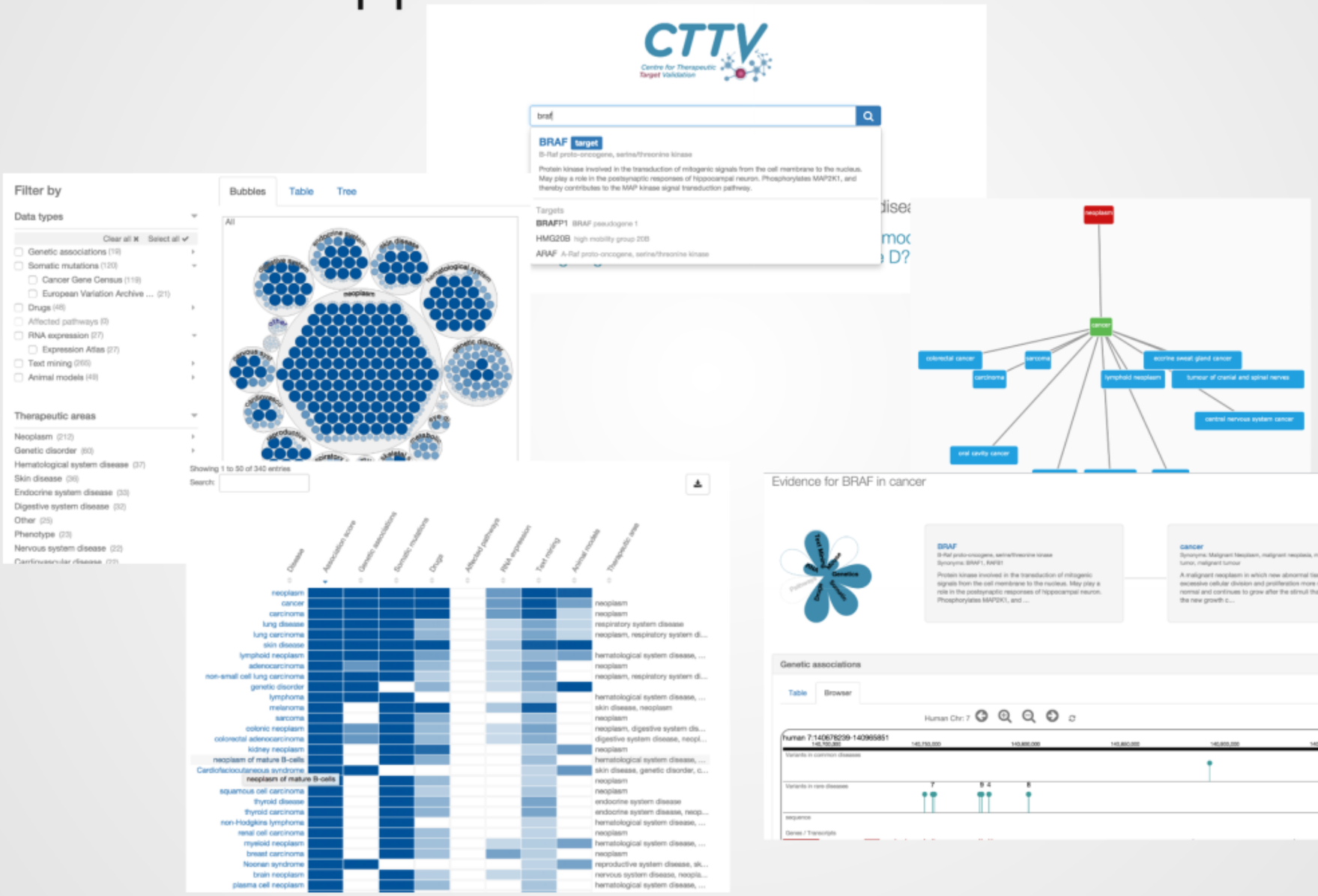

Architecture

ES Cluster

- Running in the EBI Embassy cloud (VMWare)
- CoreOS + Docker
- 3 Nodes
  - Production: 4 CPU / 12 Gb RAM / 40 Gb SSD
  - Staging: 4 CPU / 8 Gb RAM / 100 Gb spinning disk

Architecture evolution

- Migrate from 1.7.2 to 2.1
- Drop production/staging paradigm and move to one big cluster
  - hot and cold nodes
  - tagged version of the data
  - support multiple version of data / api / webapp within the same infrastructure

Summary

Elasticsearch at CTTV

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Flexible, can easily handle many types of data

Main document datastore

Backend for computational pipeline

Powering REST API and WEB APP

Potential to run on demand map reduce computation


IT WORKS!

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Core platform development team

Andrea Pierleoni

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Samiul Hasan

?