Guixifying workflow management system

Past, present, maybe future?

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Université Paris Cité

GuixHPC

3 minutes is quick!
Join the fun, **join Guix!**

Workflow?

when pipeline is more than a line of pipes

data $\xrightarrow{\text{pipeline}}$ result(s)

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zcat R1.fastq.gz | grep ATGC | sort | uniq -c
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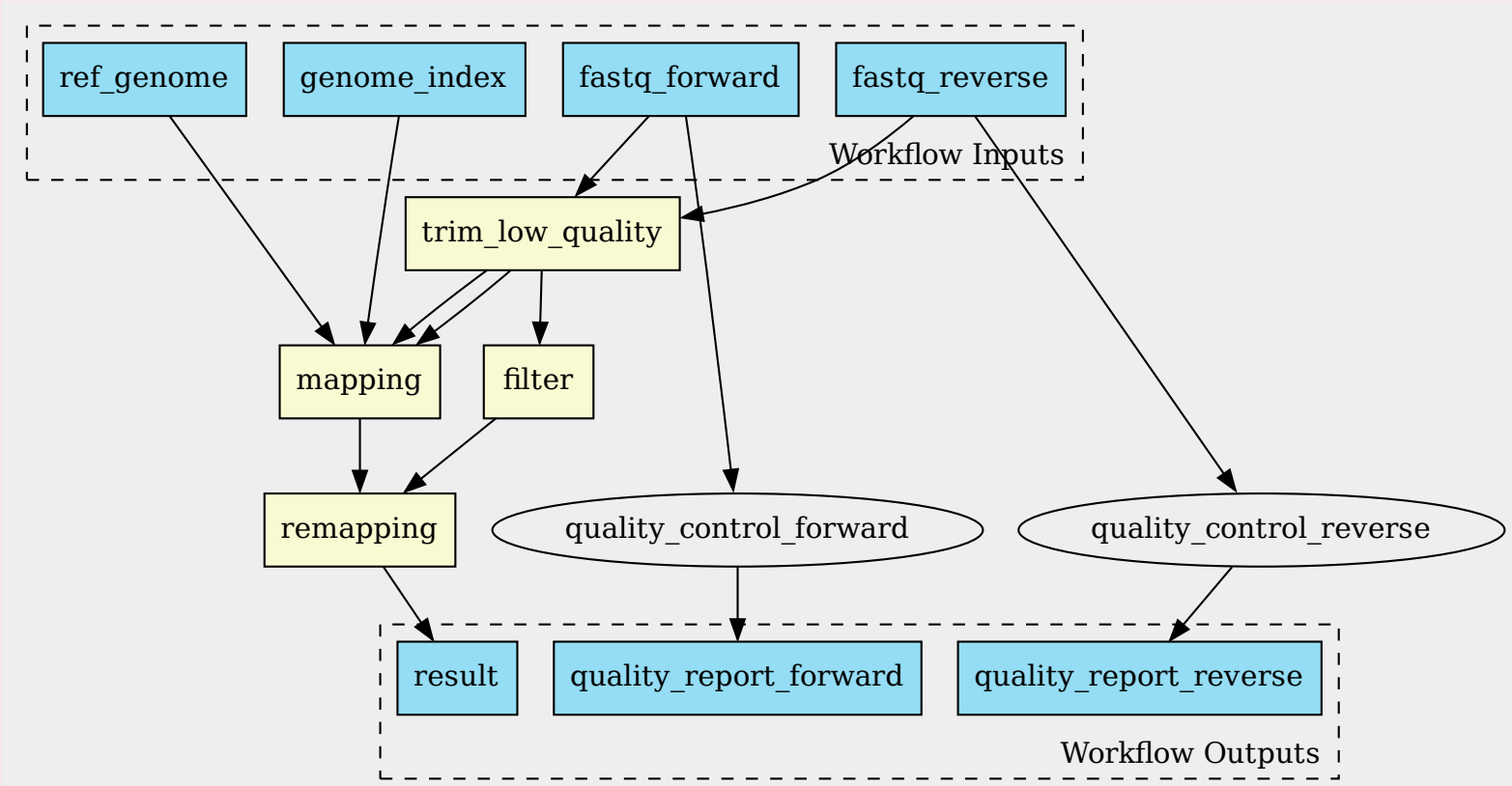

long-term reproducible workflow?

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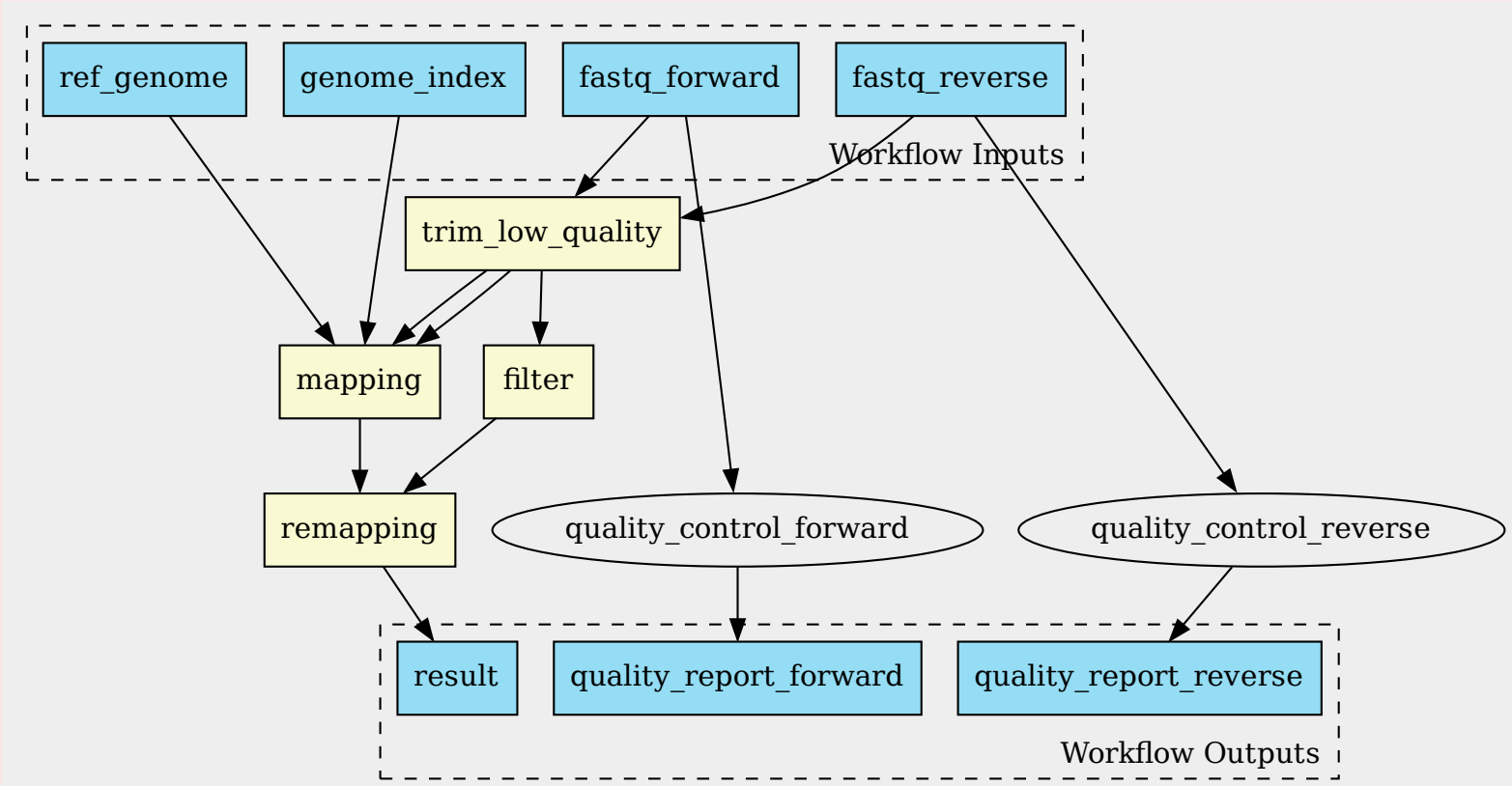

long-term reproducible workflow?

- Binaries? (each box)
- Describe such graph?

Workflow?

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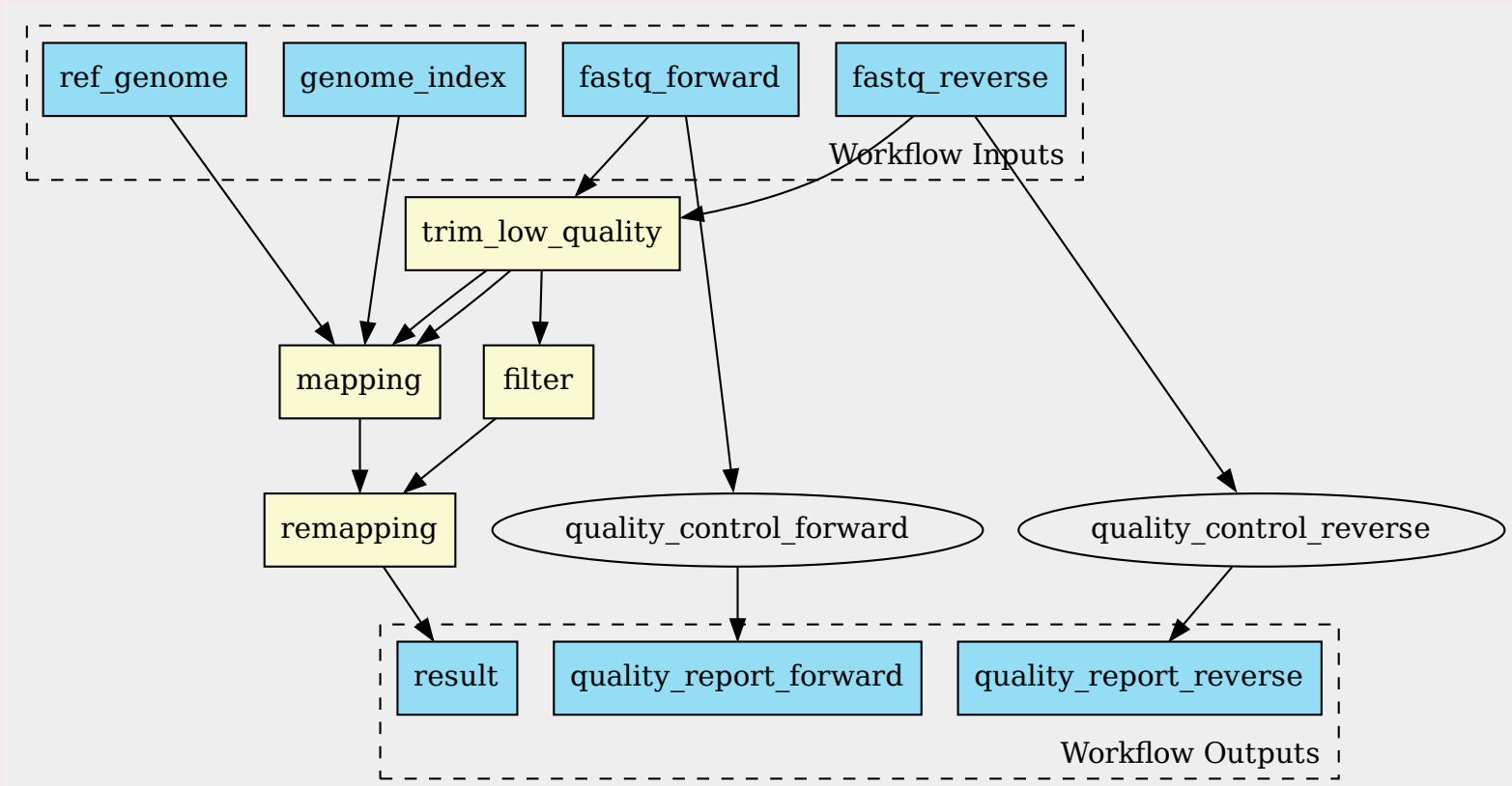

long-term reproducible workflow?

- Binaries? (each box) $\Longrightarrow$ Guix!
- Describe such graph?

Guix = *reproducible* computional environment (auto-promo)

Open Research Tools and Technology devroom (FOSDEM)

Guix, toward practical transparent, verifiable and long-term reproducible research (link) 2023

Guix + Software Heritage:
Source Code Archiving to the Rescue of Reproducible Deployment (link) 2025

one paper

Toward practical transparent verifiable and long-term reproducible research using Guix (link)

`https://hpc.guix.info`

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binaries ok!

Workflow management with Guix (link) FOSDEM 2017
Extending a reproducible software deployment system (link) FOSDEM 2021

- Package management is graph management
- Workflow is graph management
- Workflow engine on the top of the package management system

Guix as a library to provide a workflow domain-specific language

Guix Workflow Language

Roel Janssen & Ricardo Wurmus

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Guix as a library to provide a workflow domain-specific language

Adoption?

- Yet another language... and based on *(count (the (closing) (parenthesis language!)))*
- High competitive market! (Make, Snakemake, Galaxy, Nextflow)
- Too *disruptive* at the time?

Common Workflow Language implementation powered by Guix (link) FOSDEM 2025

- Common Workflow Langage = a language with a standard specification document
- It eases implementation diversity

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ravanan = yet another CWL engine implementation

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ravanan = yet another CWL engine implementation

but powered by Guix!

`https://github.com/arunisaac/ravanan`

Time's up!

Concise Common Workflow Language — Arun Isaac

Concision and elegance in a workflow language using Scheme (link) FOSDEM 2022

Because *(count (the (closing) (parenthesis language!)))* rocks!

Using Guix for producing containers

```
guix pack -f docker -m manifest.scm
```

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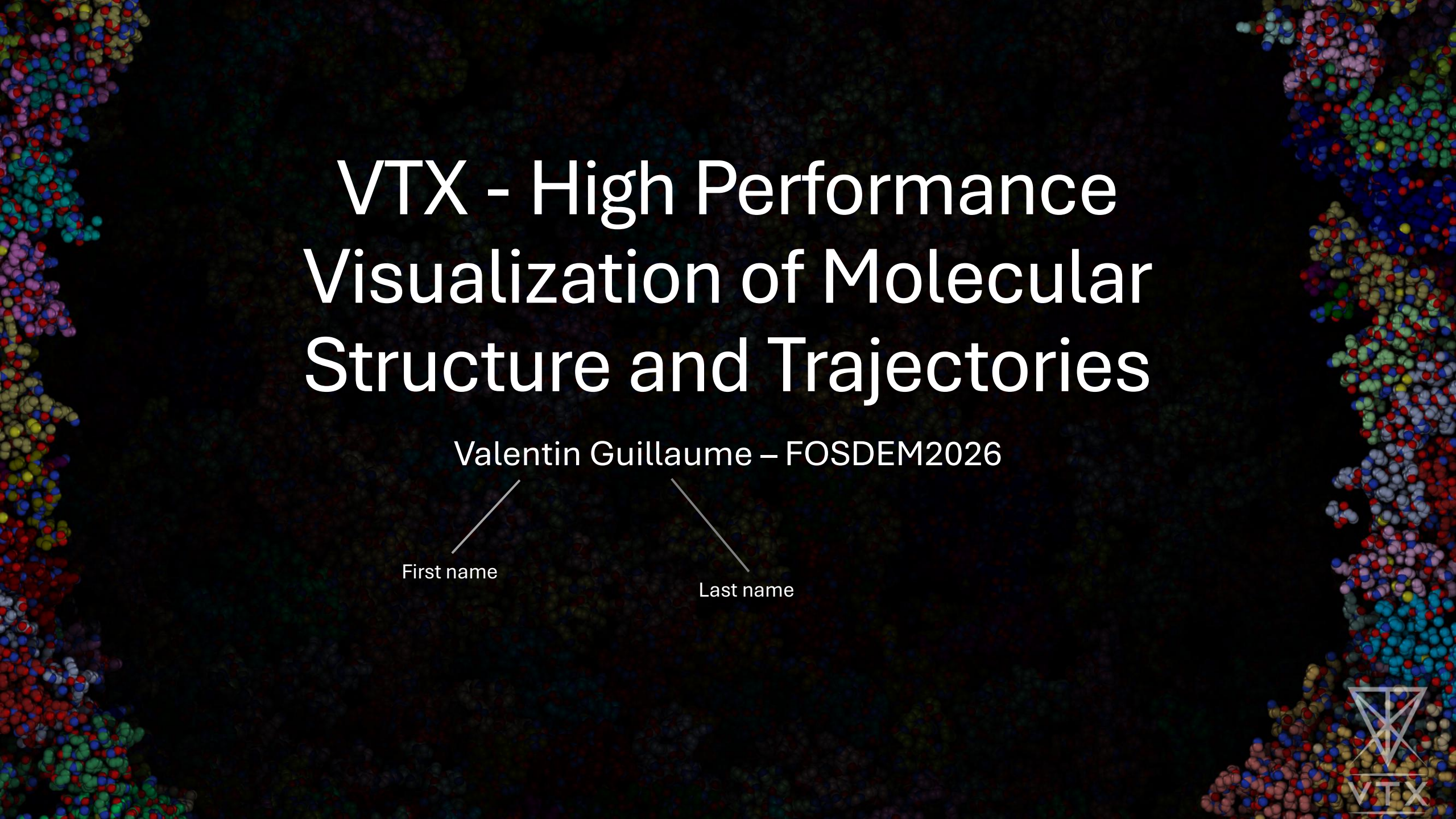
Let me know your story about **long-term reproducible workflow**

VTX - High Performance Visualization of Molecular Structure and Trajectories

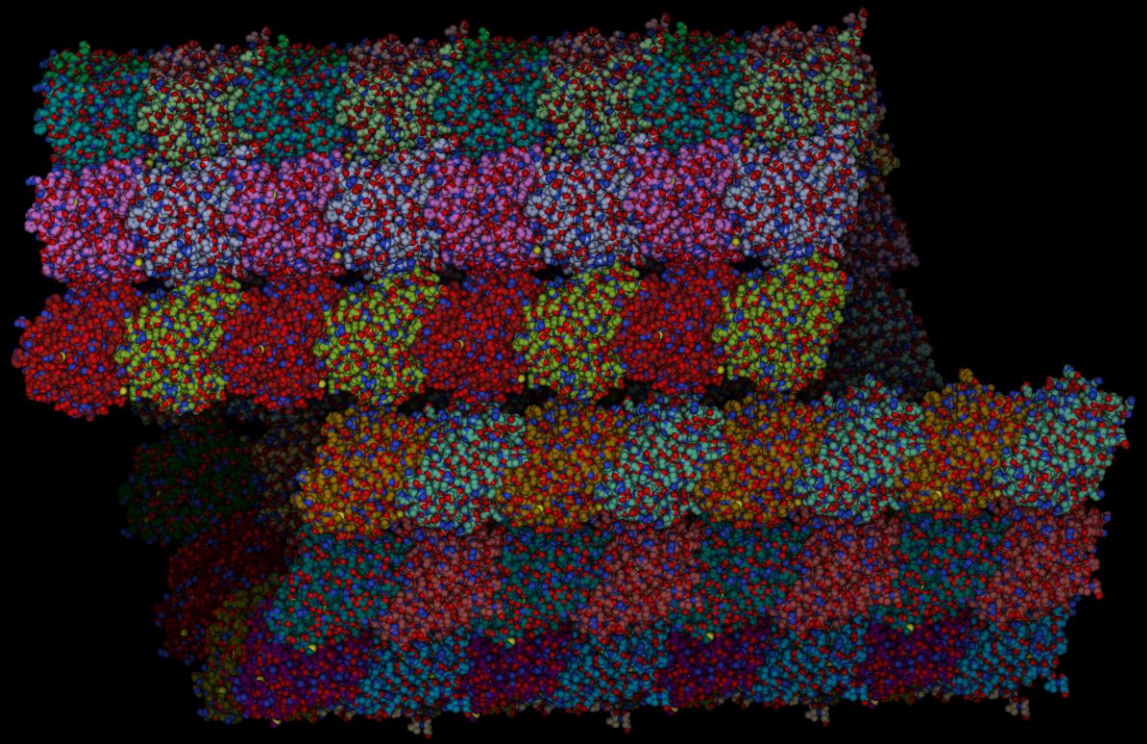
Valentin Guillaume – FOSDEM2026

First name

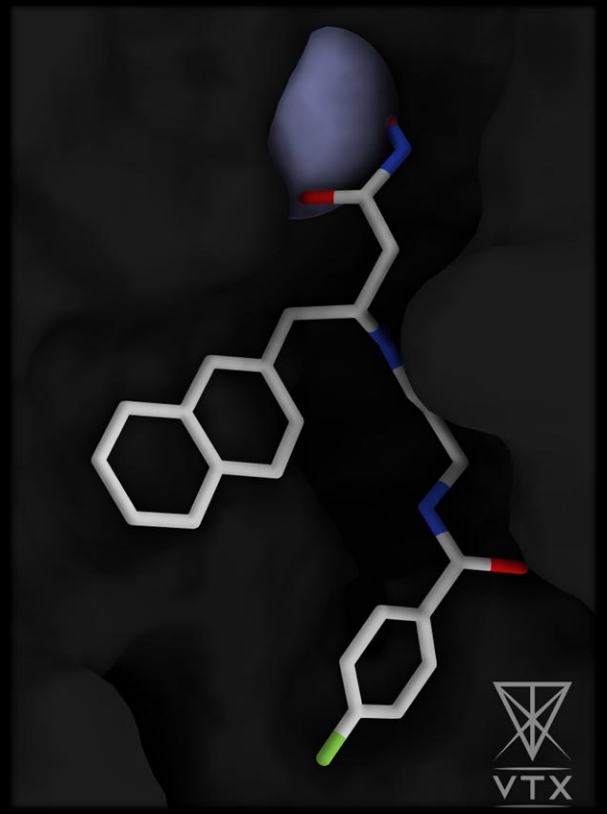
Last name



Why do we need a visualization software ?



Understanding protein-protein interactions



Designing drugs

Yet another one ?

Case study :

Coarse grained whole-cell Martini model of JCVI-syn3A :

114 million Martini beads

- 60,887 soluble proteins
- *2,200 membrane proteins*
- *503 ribosomes*
- a single 500 kbp circular dsDNA
- *1.3 million lipids*
- 1.7 million metabolites
- 14 million ions

(Stevens et al, Front. Chem 2023)

Yet another one ?

Performance matters.

software	Frame per second for this ~100M beads system (on this very laptop)
Pymol	Crashes
ChimeraX	Freezes
VMD	1.4 frame/s
VTX	12 frame/s

Designed for big systems

.. visual matters too.

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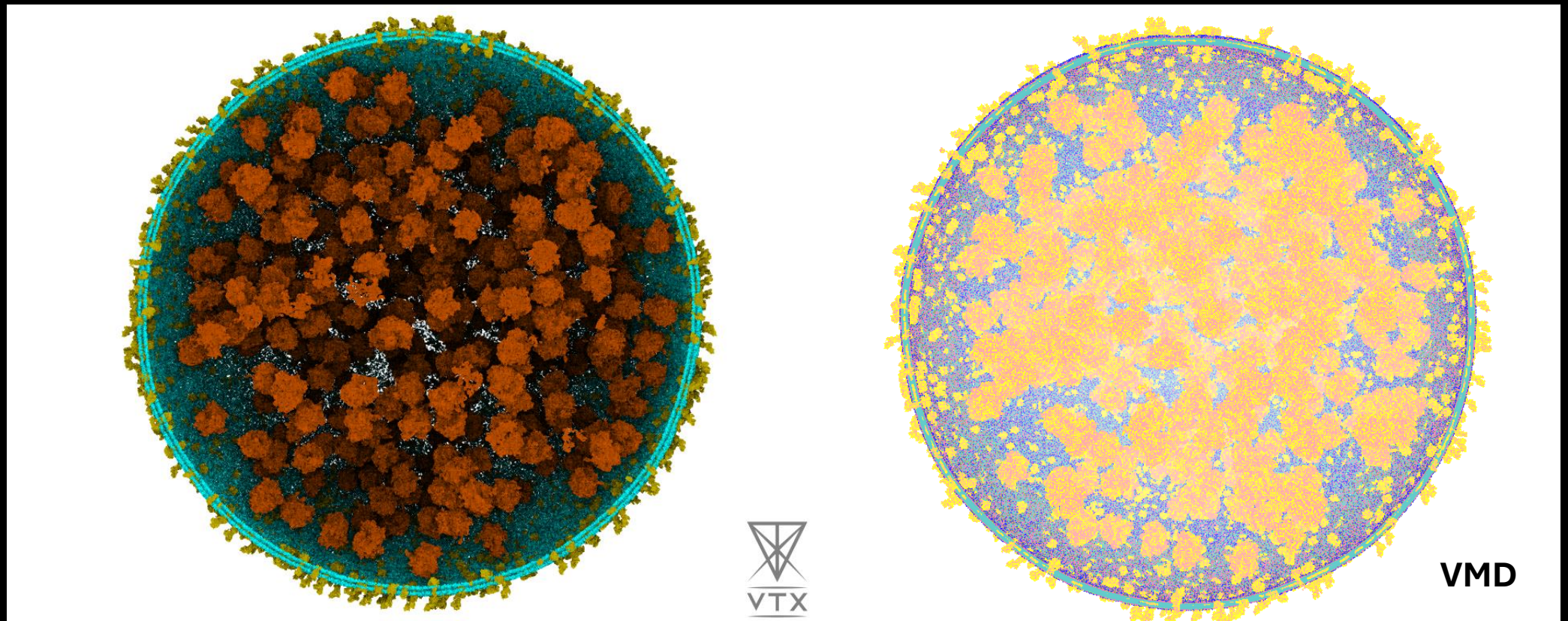
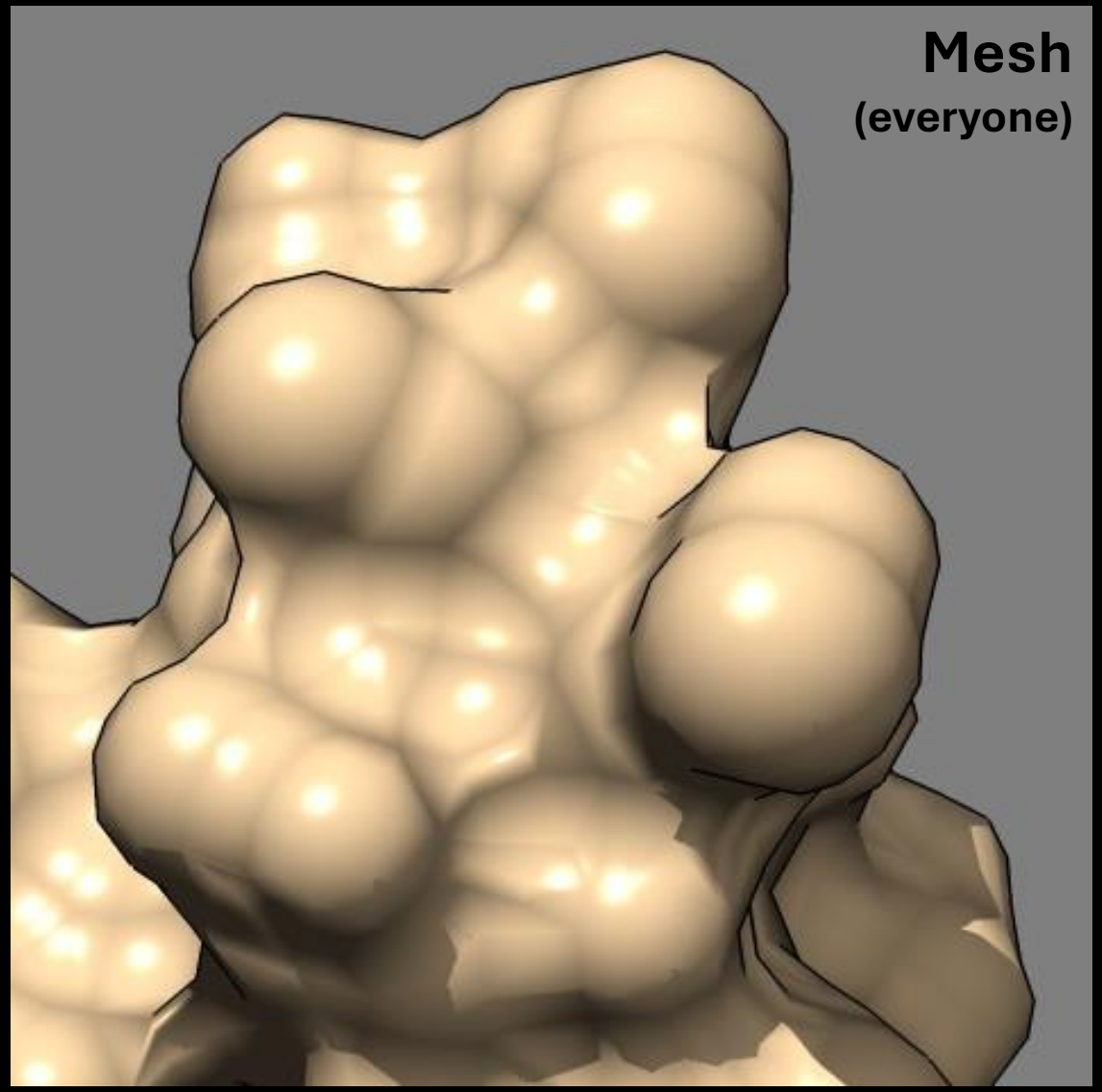
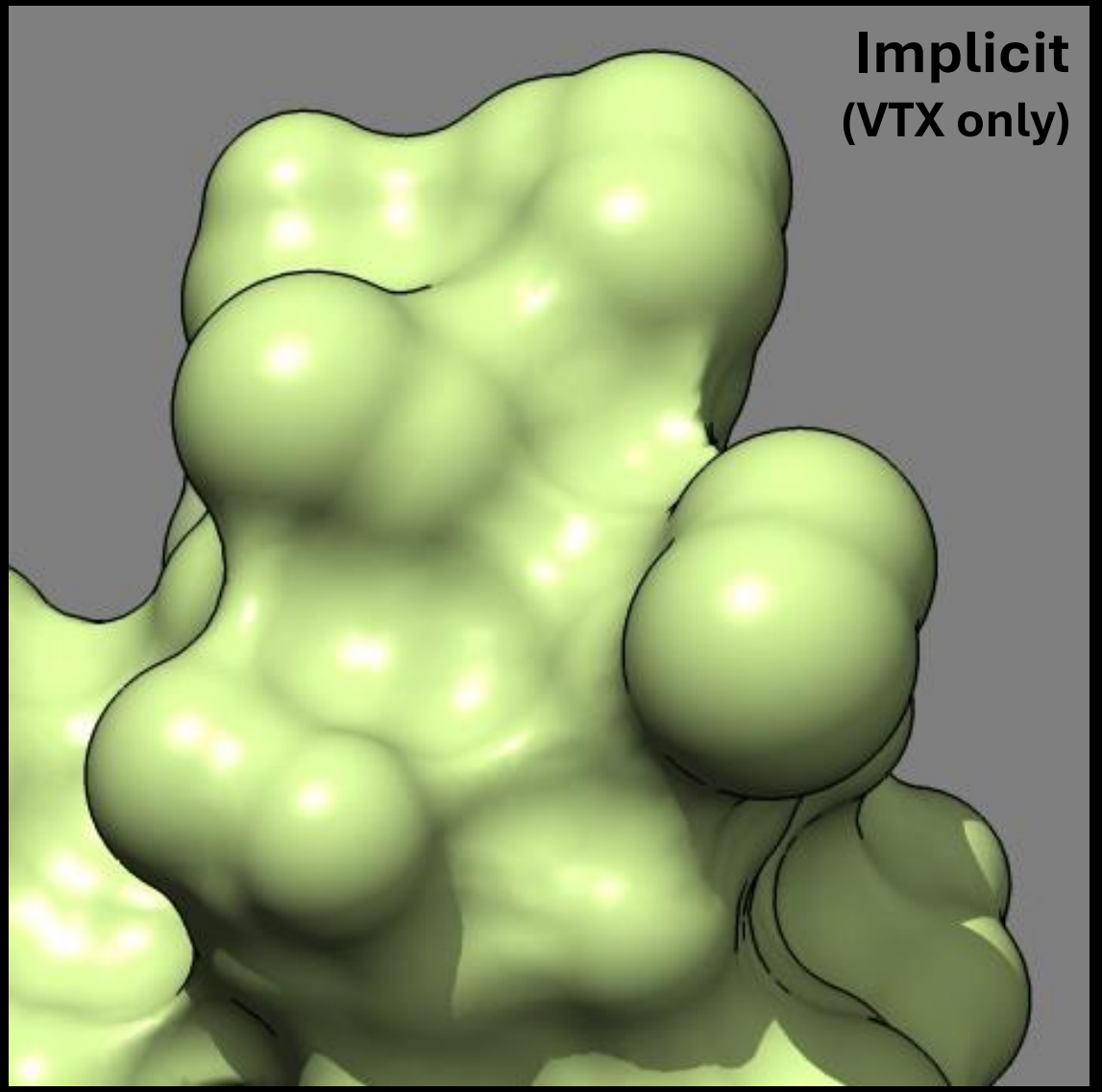


Upcoming version : Meshless Solvent Excluded Surface





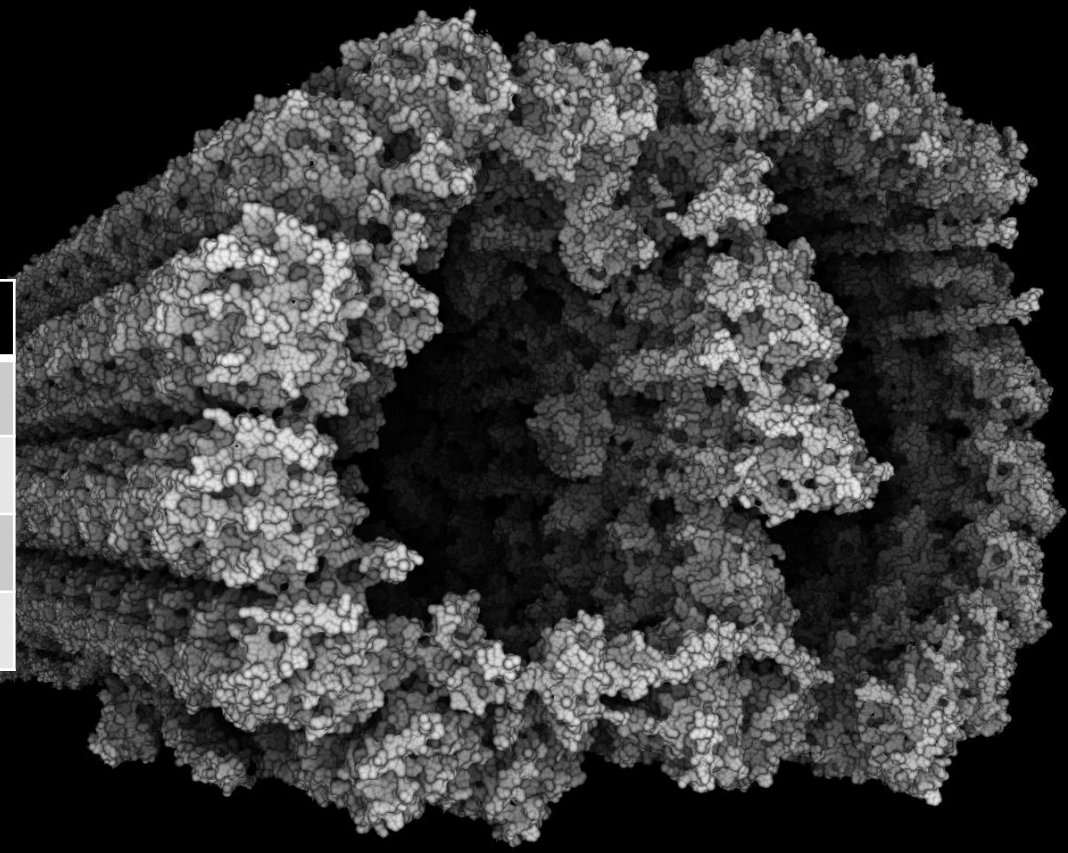
pixel perfect quality

Meshless Solvent Excluded Surface

Performances ?

PDB id	# Atoms	Mesh		Meshless (VTX)	
		Time (ms)	Mem (MB)	Time (ms)	Mem (MB)
1AGA	126	4.5	11.9	3.22	0.39
7RGD	65008	16.86	6123	18.06	214
3J3Q	2440800	-	-	700.17	7631

(Plateau-Holleville, 2024)



pixel perfect quality + fast rendering

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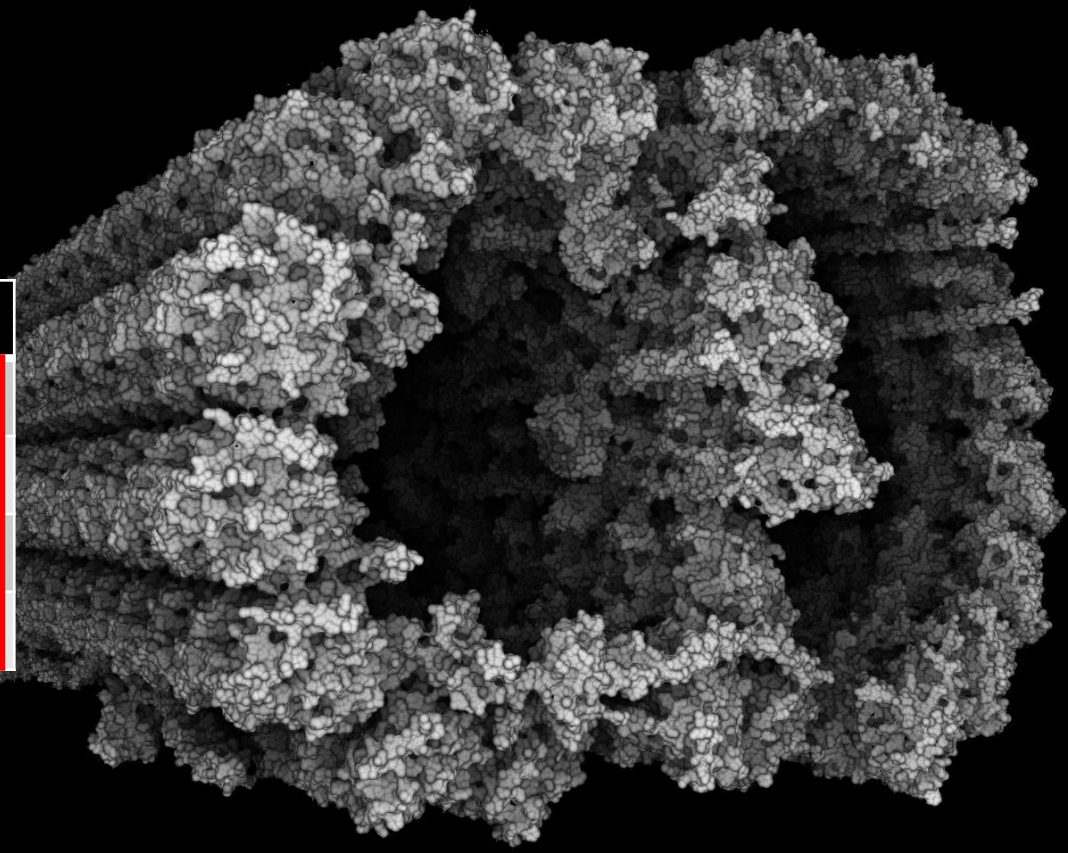
Not enough VRAM



pixel perfect quality + fast rendering + reduced memory usage

Take away - VTX

- Already available (scan QR code)
- High performance visualization
- Meshless representation (SES in next version)
- Open source (come and contribute !)

http://vtx.drugdesign.fr

Mail me at **valentin.guillaume@lecnam.net**

Bridging cutting-edge structural bioinformatics, computer graphics and video game interaction

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IUF

le cnam

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M2D2

xlim INSTITUT DE RECHERCHE

M. Maria, V. Larroque C. Plateau-Holleville

cedric G. Levieux

LCT Laboratoire de Chimie Théorique JP. Piquemal

Qubit PHARMACEUTICALS Y. Naimi

rijksuniversiteit groningen J Stevens SJ. Marrink

VTX

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@VTX_mol

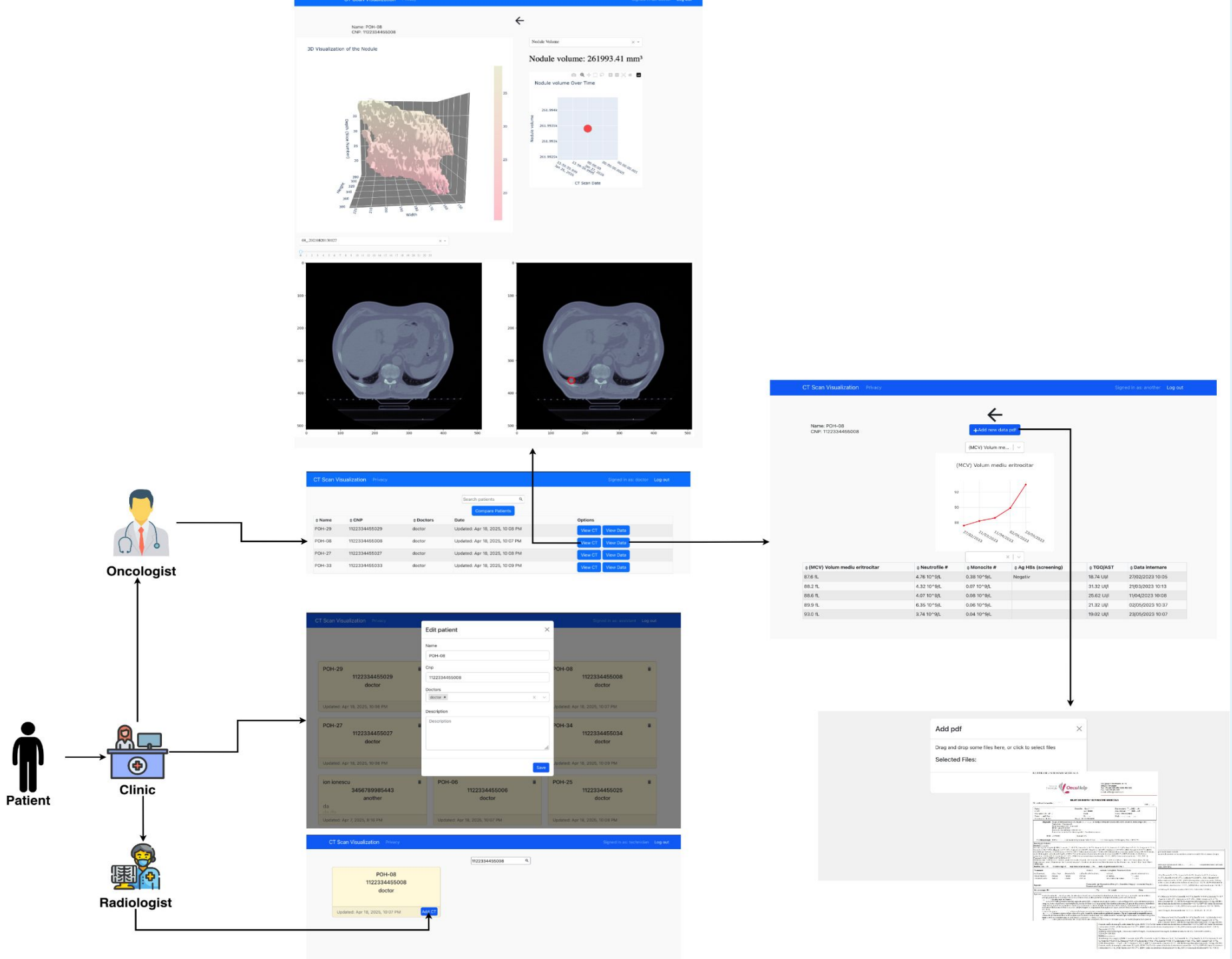
Multimodal Tumor Evolution Analysis: Interactive 4D CT and Time-Aligned Clinical Data in a Hospital Web Platform

Bioinformatics & Computational Biology , FOSDEM'26
January 31, 2026

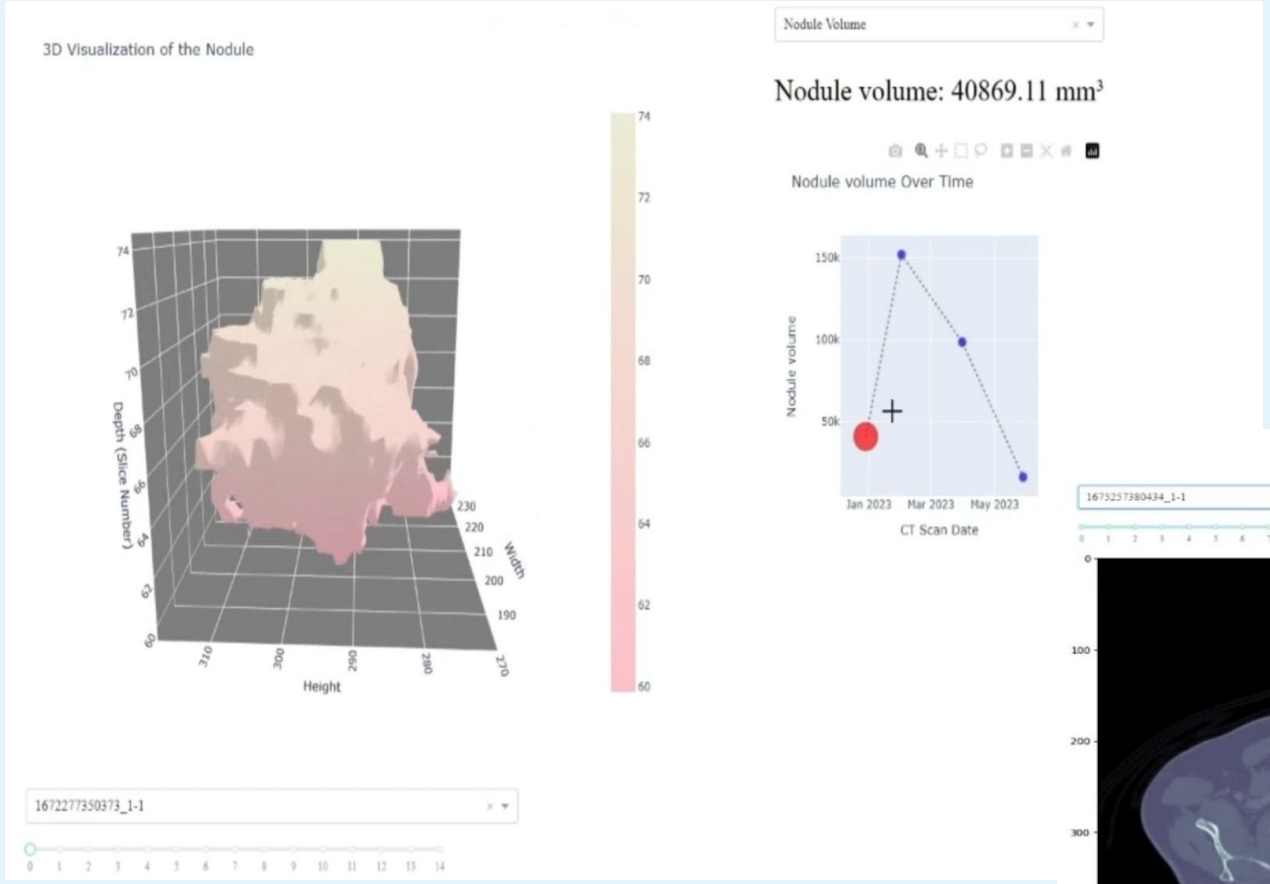
About

- Fabian Fulga
- PhD Student
- Research Assistant
- Github: @fabi200123
- Email: fabian.fulga@upt.ro

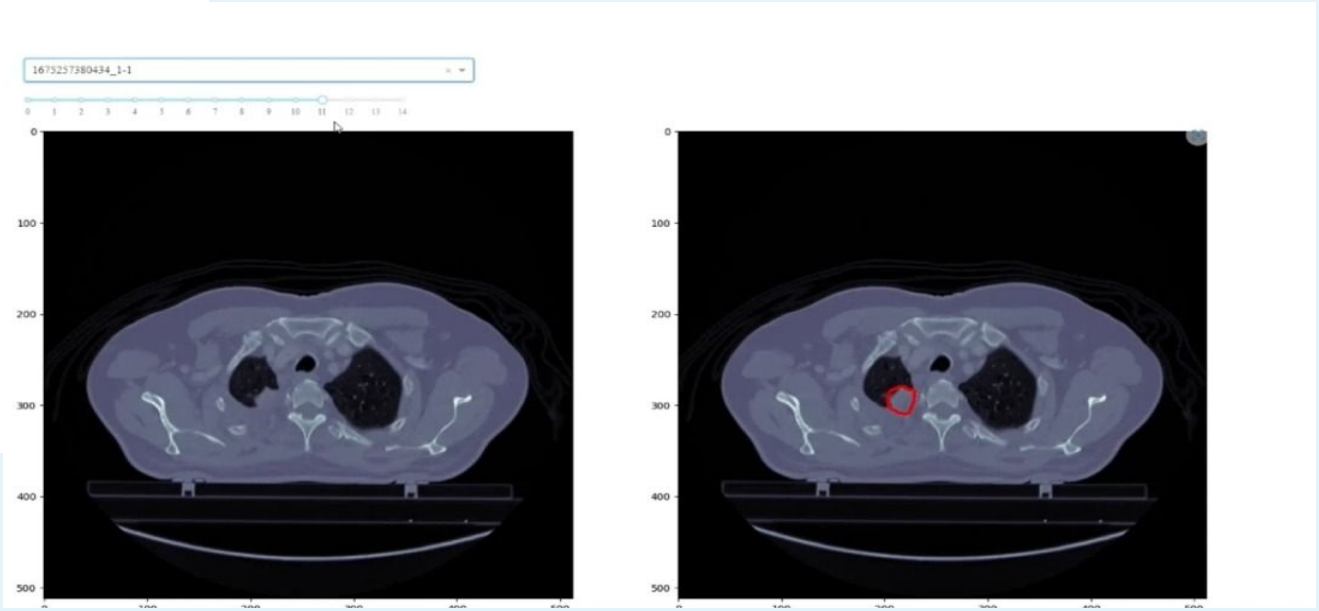
Introduction



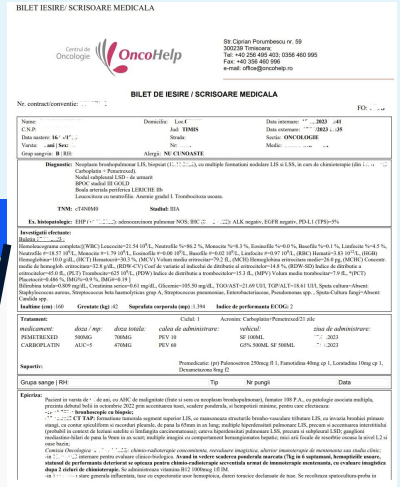
Nodule visualization



- based on **Precision-medicine-toolbox**
- **Pyradiomics** for extracting characteristics

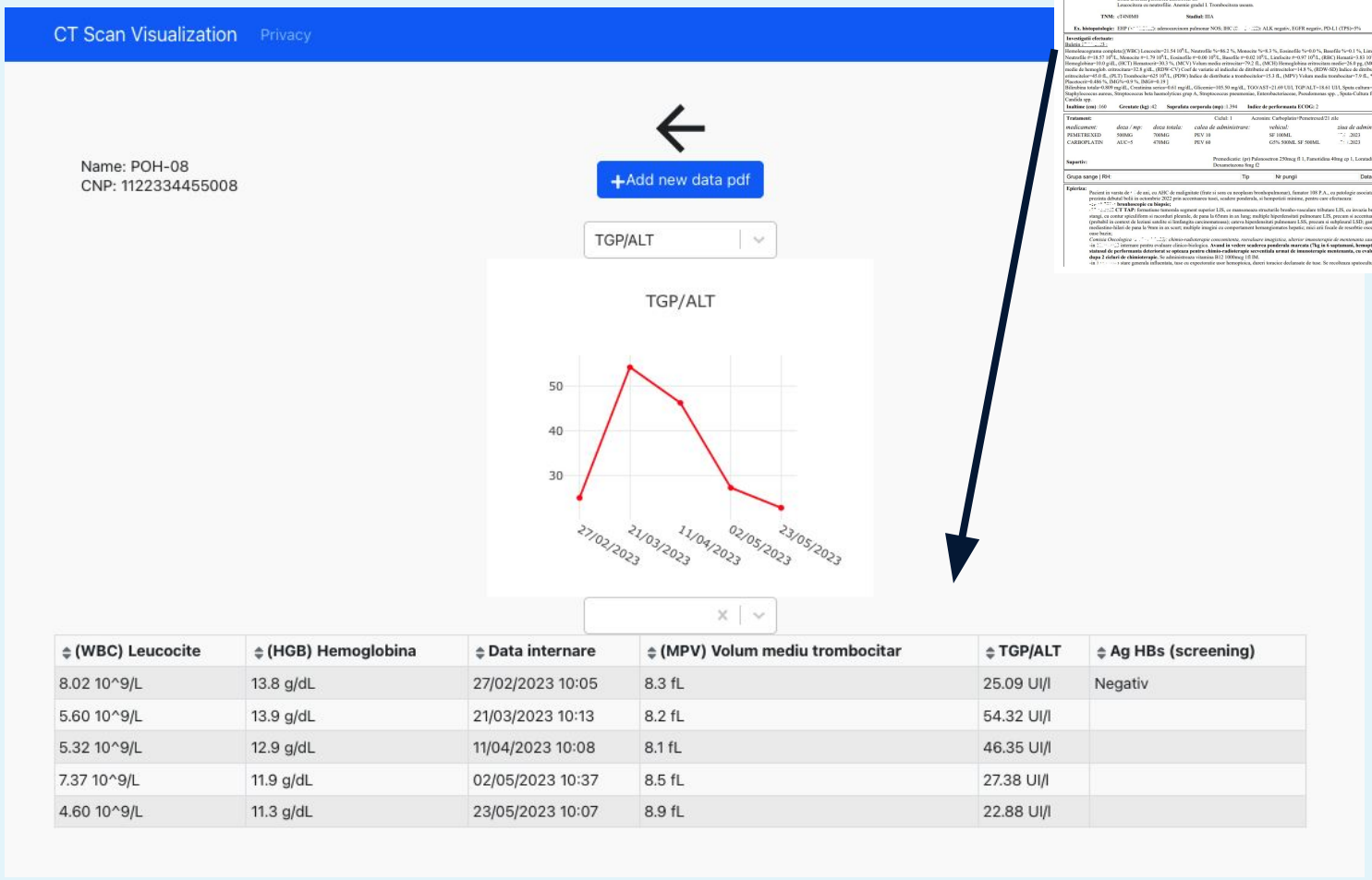


Data visualization


BILET IESIRE/ SCRISOARE MEDICALA

OncoHelp

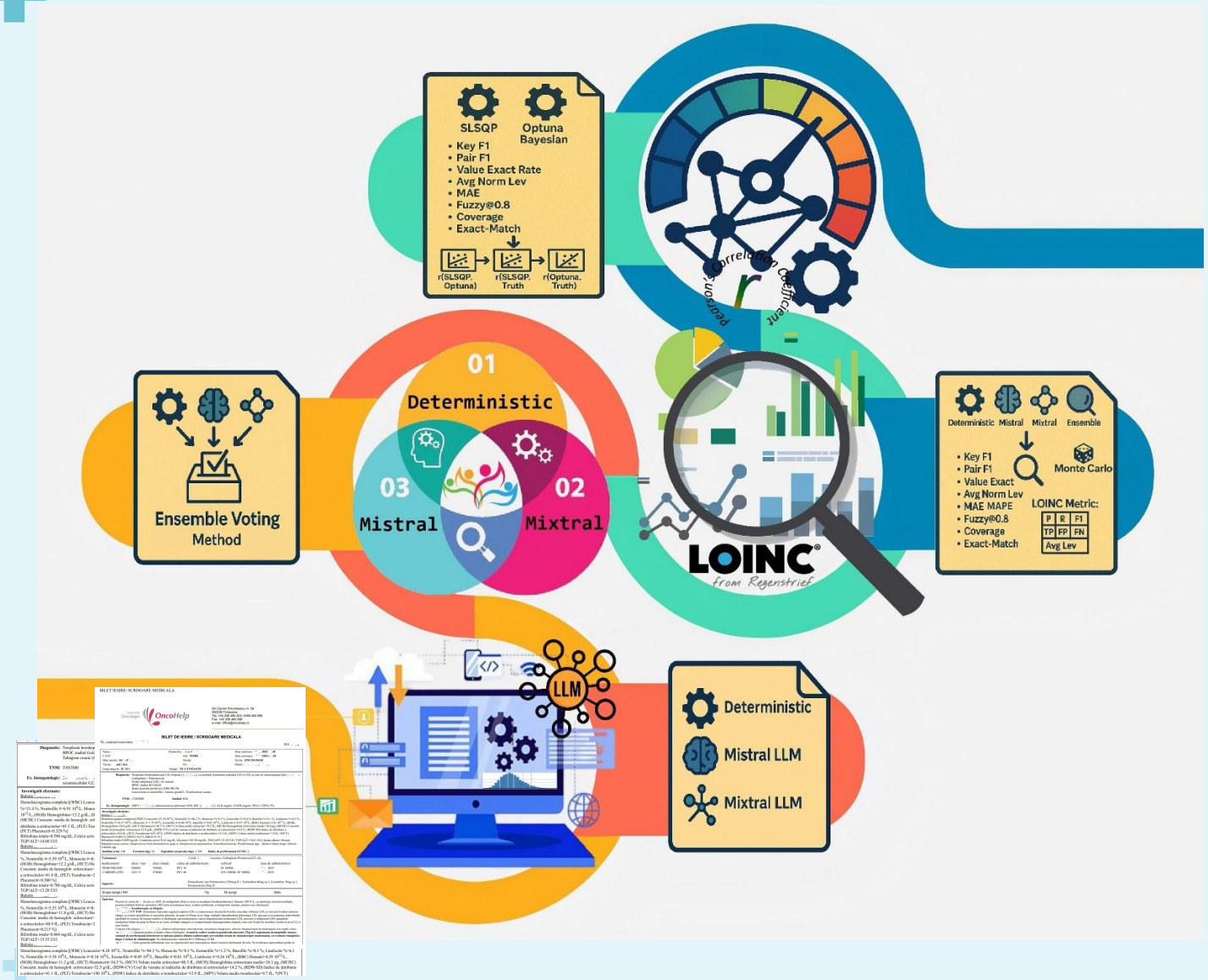
BILET DE IESIRE / SCRISOARE MEDICALA



(WBC) Leucocite	(HGB) Hemoglobina	Data internare	(MPV) Volum mediu trombocitar	TGP/ALT	Ag HBs (screening)
8.02 10^9/L	13.8 g/dL	27/02/2023 10:05	8.3 fL	25.09 UI/l	Negativ
5.60 10^9/L	13.9 g/dL	21/03/2023 10:13	8.2 fL	54.32 UI/l	
5.32 10^9/L	12.9 g/dL	11/04/2023 10:08	8.1 fL	46.35 UI/l	
7.37 10^9/L	11.9 g/dL	02/05/2023 10:37	8.5 fL	27.38 UI/l	
4.60 10^9/L	11.3 g/dL	23/05/2023 10:07	8.9 fL	22.88 UI/l	

- Interactive view of discharge letters
- Graphical evolution over time
- Customizable and interactable table

Data extraction



- PDFs are parsed by 3 models
- Scores are extracted comparing the results with the ground truth
- Voting algorithm to select best output to add patient data

Github Repositories

- Web platform: https://github.com/owtlaw6/Licenta
- CT Visualization: https://github.com/fabi200123/4D_CT_Scan
- Full tool: https://github.com/fabi200123/Nodule-Data-Visualizer

DNA storage and open-source projects

Babar Khan, FOSDEM 2026

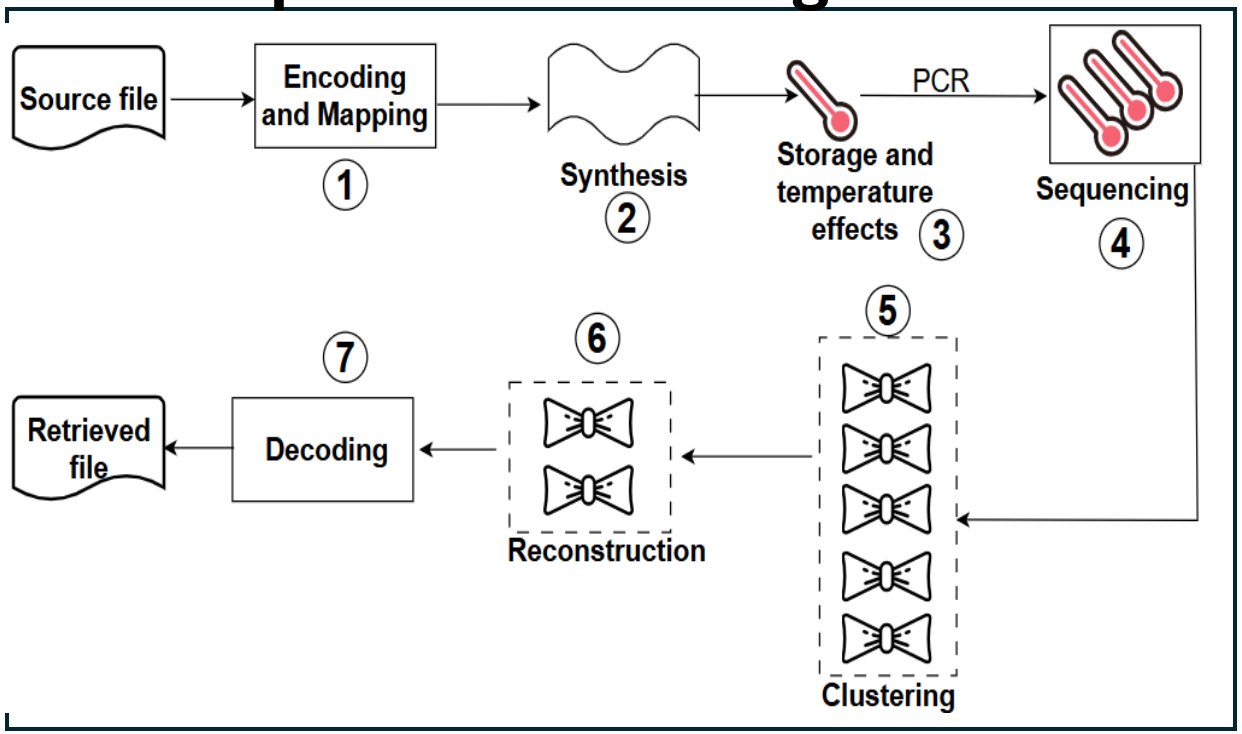
Data growth as of now

In 2025:
175 Zettabytes

What does it mean?

200 trillion DVD movies
OR
4 billion 16-TB drives

7 steps of DNA storage



What does it mean?

- Store data for 2000 years
- Store Wikipedia in test tube

Want to learn more about DNA storage?

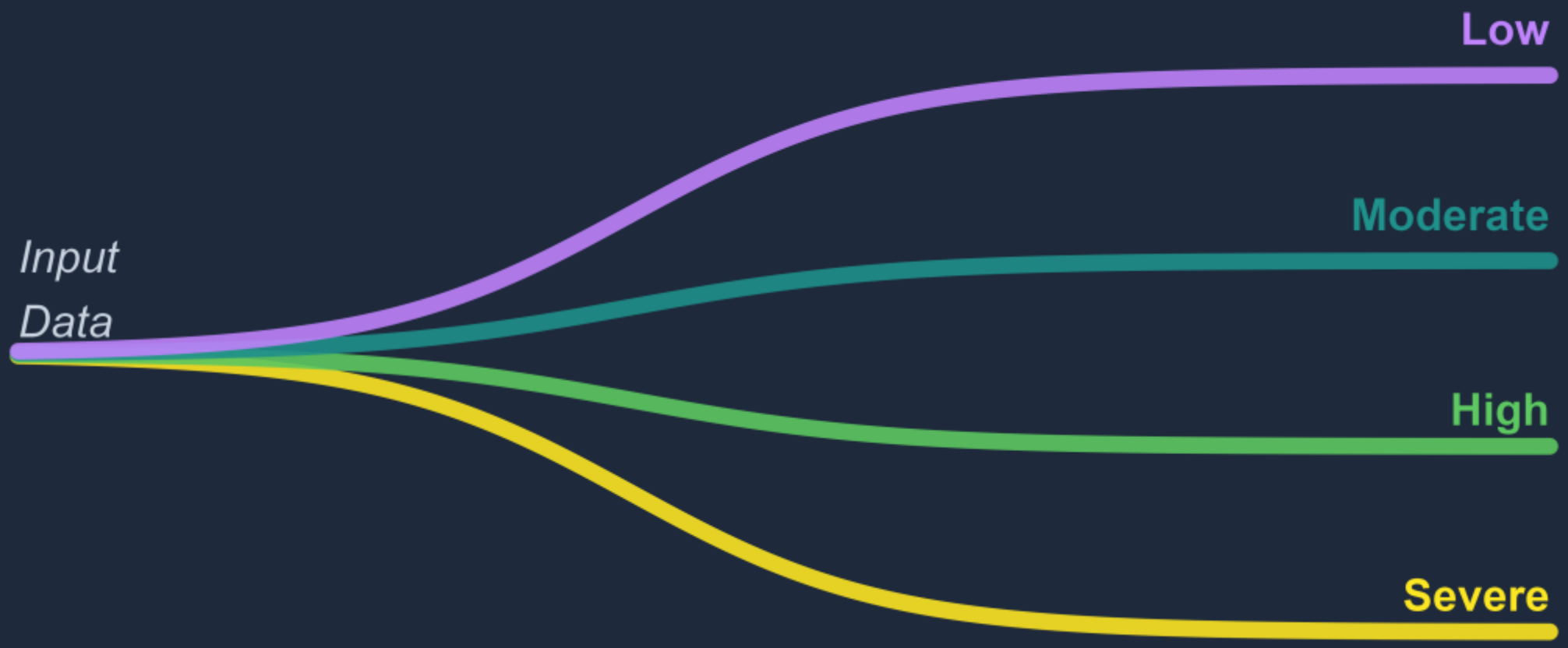
Answer: scan/fork/star **awesome-dna-storage** github repository

BabarZKhan/awesome-dna-storage: curated list of dna-storage resources

OptSurvCutR

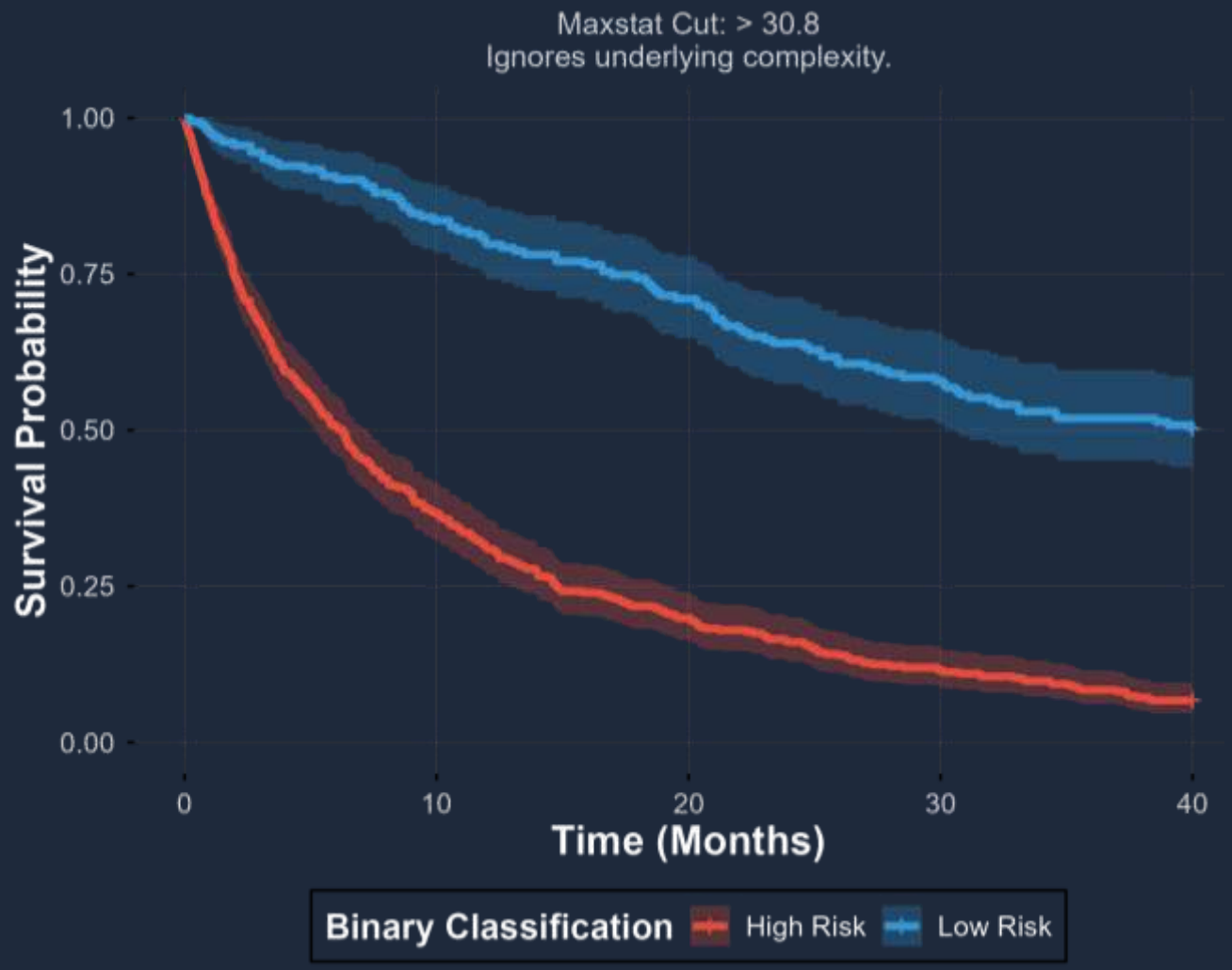
Automating Multi-State Survival Discovery

Payton Yau



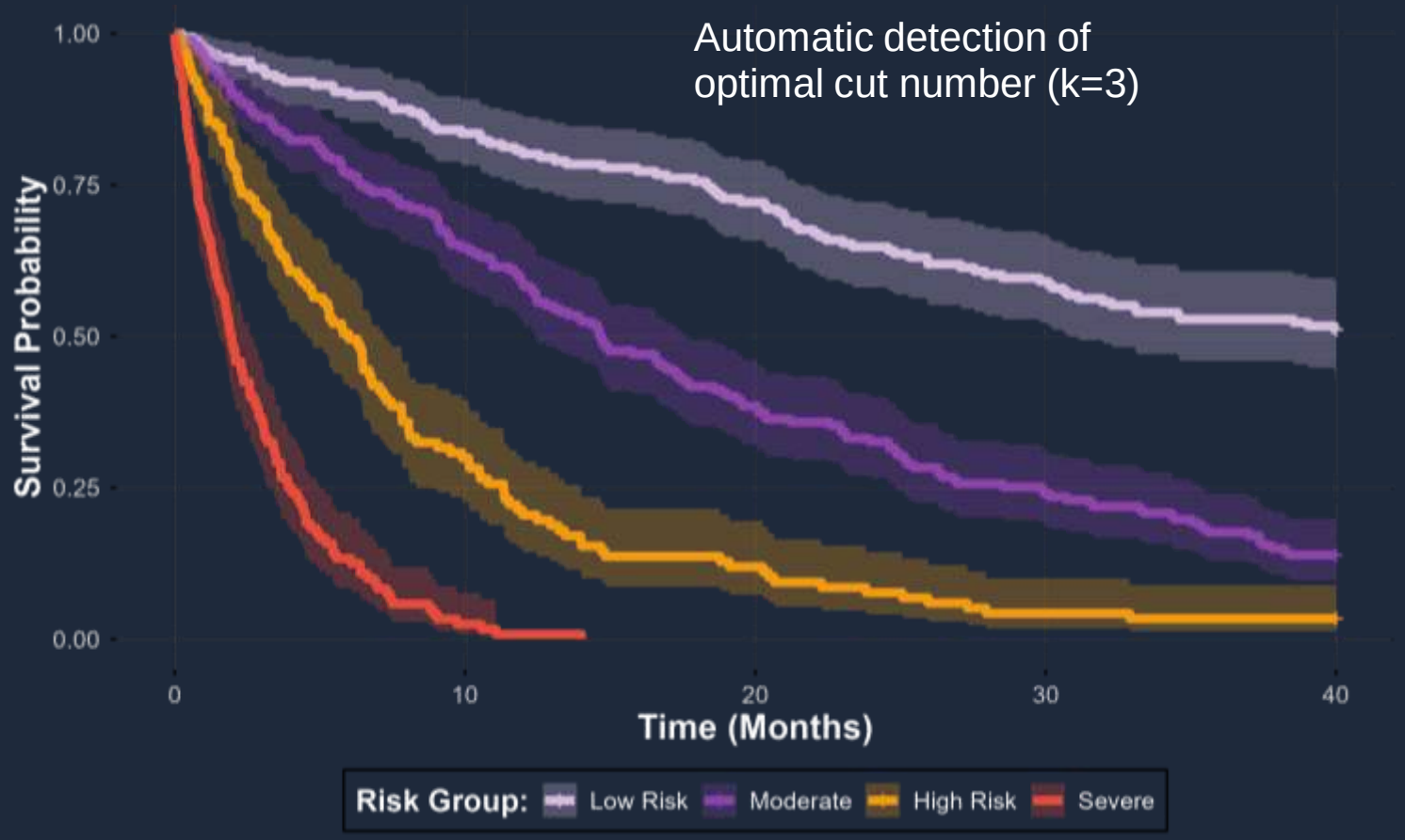
FOSDEM | Bioinformatics DevRoom

Biology is a Gradient, Not a Switch



≠

Detecting the Gradient: Automated Multi-State Discovery



Systematic scan for multiple thresholds

Identifies 3, 4, or 5+ risk strata

Captures non-linear risk profiles (e.g., U-shape)

1. SELECT k → **2. OPTIMISE** → **3. VALIDATE**

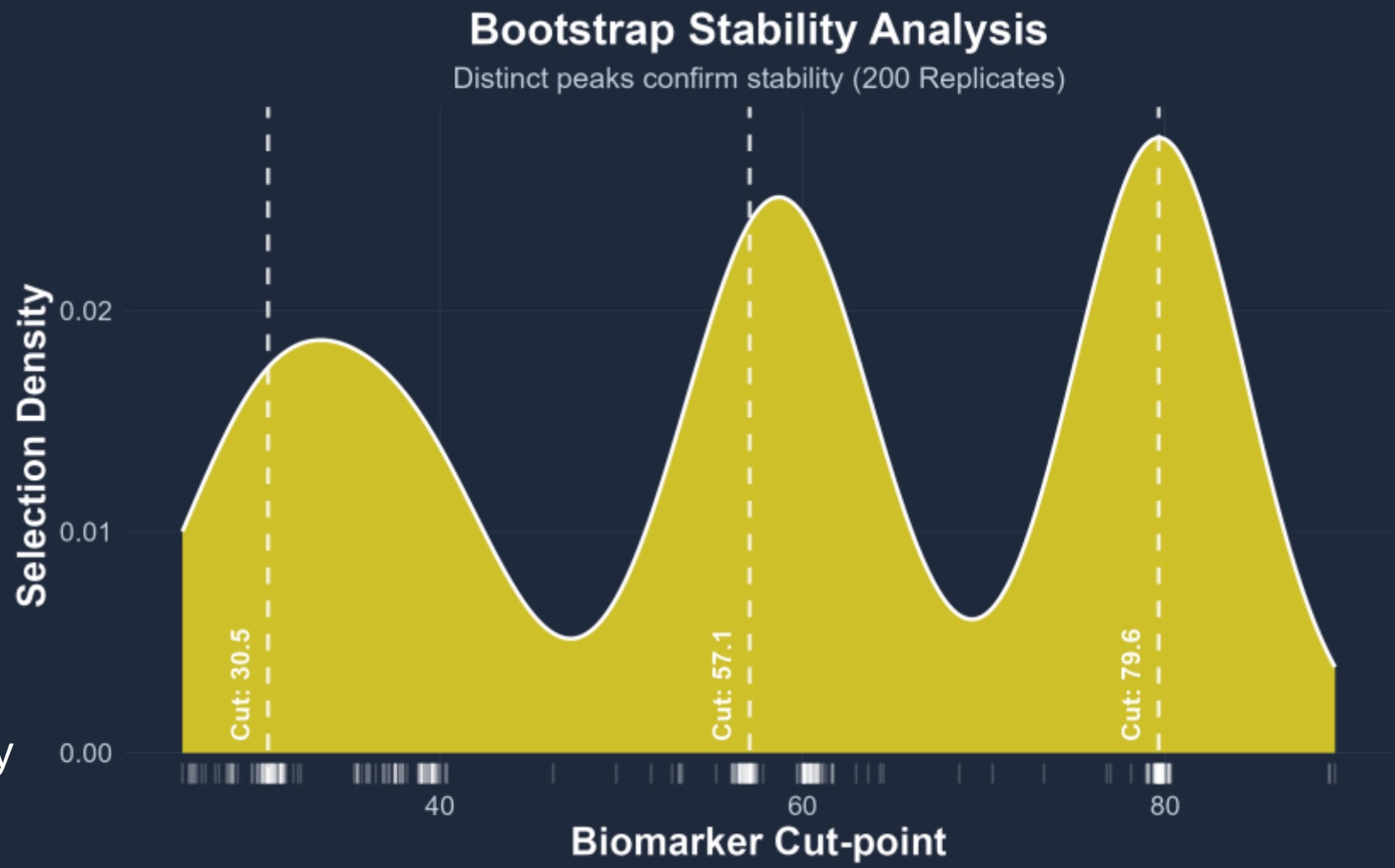
AIC/AICc/BIC *MSRS* *Bootstrap*

Signal *vs.* Noise: Rigorous *P-Value* Correction

PROBLEM ⚠
Uncorrected *P-values* →
False Positives (Type-I Error)

SOLUTION ⍰
Maximally Selected Rank Statistics (MSRS)

CONFIRMATION 🔁
Bootstrap resampling to verify stability



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AIC/AICc/BIC

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MSRS

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Bootstrap

OptSurvCutR: High-Resolution Survival Analysis

Open Source • Reproducible • In Review

ROpenSci

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R consortium