



# 10th EUM 2025 Jülich

## EasyBuild @ Fred Hutch

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March 25, 2025

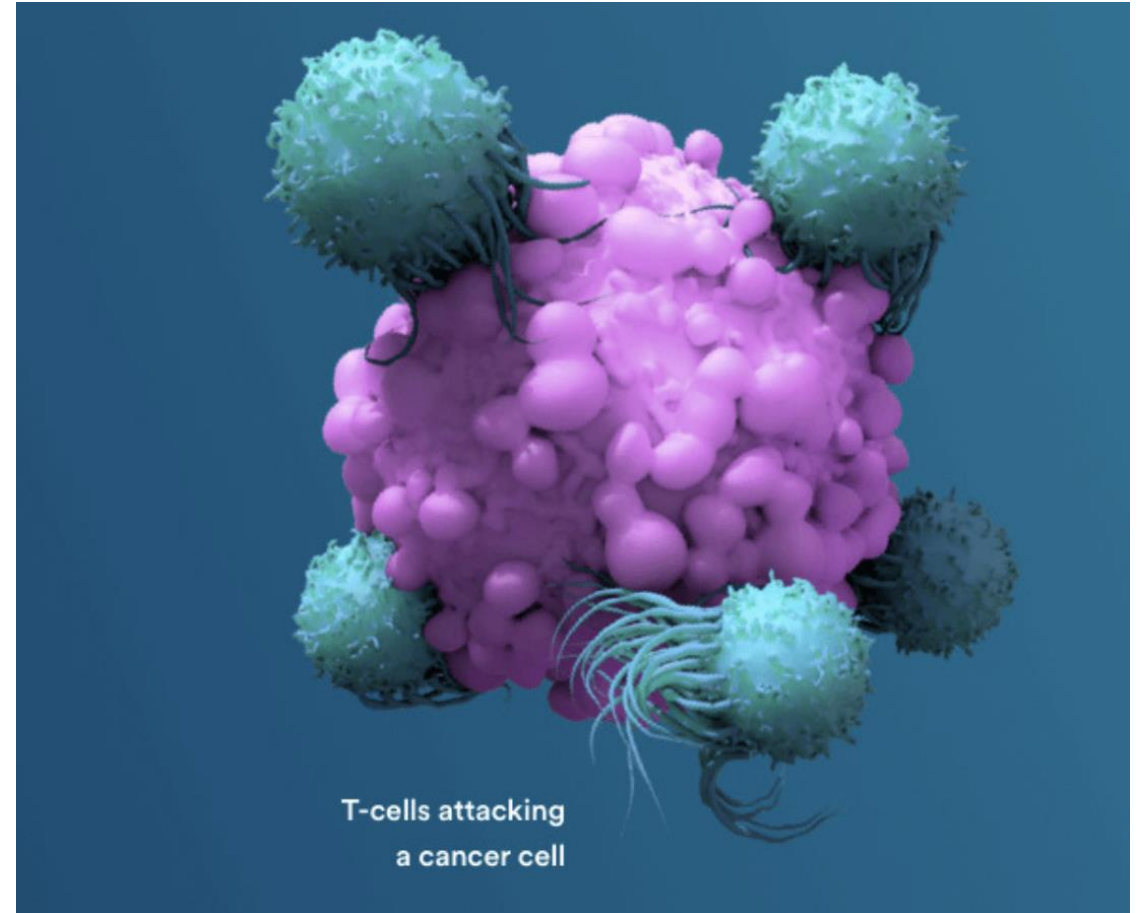
# Fred Hutch Cancer Center Profile

Developing Immunotherapies  
for treating Cancer

Cancer Research Center with On-Site Clinical  
About 300 Principal Investigators

Graduate Student and Postdoctoral Training

Home to 3 Nobel Laureates  
50<sup>th</sup> Anniversary of the Center





# Scientific Computing @ Fred Hutch

14 Nodes GPUs deployed Q3 Ubuntu 24.04 Zen4 4x L40S GPUs

174 Node cluster deployed during 2020

- Slurm - Ubuntu – Intel dual socket 36 Cores - 748 GB – Single GPU RLX 2080
- 4.7 PB BeeGFS Dedicated Scratch

4 LMOD repos Bionic/Haswell, AVX512 and Zen3 Noble with Zen4

Cluster (mostly) Relies on EasyBuild / Lmod for all software

Cluster Nodes are deployed with a minimal OS install

Apptainer installed on all nodes

SciComp - Docker Swam

Open On Demand coming soon

# Module Usage from LMOD Load

R	: 3,037,280 (29.74%)	AlphaFold	: 82,887 (0.81%)
fhR	: 2,747,192 (26.90%)	CUDA	: 78,344 (0.77%)
GCC	: 525,462 (5.15%)	scikit-learn	: 71,677 (0.70%)
Boost	: 442,125 (4.33%)	Anaconda3	: 55,393 (0.54%)
Eigen	: 442,038 (4.33%)	fhSeurat	: 52,516 (0.51%)
Python	: 372,861 (3.65%)	gdc-client	: 50,068 (0.49%)
BCFtools	: 328,022 (3.21%)	Bowtie2	: 42,568 (0.42%)
BEDTools	: 272,528 (2.67%)	TensorFlow	: 39,252 (0.38%)
Apptainer	: 198,291 (1.94%)	Java	: 34,169 (0.33%)
Biopython	: 158,434 (1.55%)	MACS2	: 26,411 (0.26%)
libiconv	: 147,036 (1.44%)	VEP	: 25,924 (0.25%)
SAMtools	: 118,397 (1.16%)	PyTorch	: 24,472 (0.24%)
GSL	: 102,828 (1.01%)	STAR	: 22,681 (0.22%)
cuDNN	: 101,770 (1.00%)	fhPython	: 18,470 (0.18%)
ImageMagick	: 100,990 (0.99%)		
GATK	: 100,218 (0.98%)		

# Tracking EasyBuild tickets

140 EasyBuild related tickets in the last year

- Tracking Types of Software Tickets new-pr, update, question, notable2build
- New-pr ticket requests
- de novo Module Requests
- Not able to build with EB – CaSpER, SCimilarity,

Use container for building software <https://github.com/FredHutch/EBcb>

Modules for Commercial Software

- ParseBioSciences SplitPipe

Containerizing Software

- AlphaFold3 with Apptainer

# User trends at Fred Hutch

Requests to use Modules with

- VS Code ( R and Python)
- RStudio-Server
- Python venv (why is Pythonpath not used by venv?)
- Seurat and Jupyter Lab

More Container Requests

How many SIF files?

GPU Usage Continues to grow

AI – scGPT

Coming Soon – Open On Demand

Ebcb – Container Build Environment for Easybuild

# Update on Easy\_Update

Please get the Latest Version 2.3.1

## **CRAN** Comprehensive R Archive Network

- EasyUpdate for R is stable and has not changed for years
- CRAN and Bioconductor is specific to each Major Minor release of R
- Bioconductor metadata Packages JSON

## **PyPI**

- Static Validation
- Pypi is getting better – pyproject.toml
- packaging.META to validate PEP 508

# EasyUpdate dep tracking with verbose

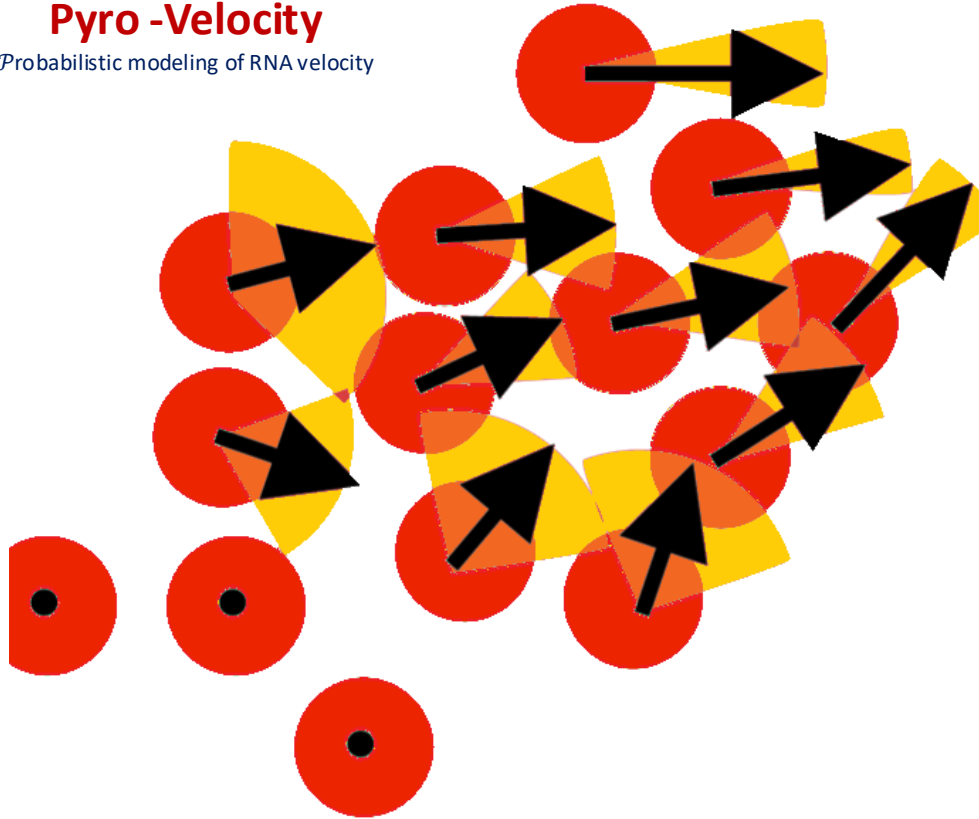
```
collections : 0.3.7 Imports from EpiModel          (add) [730, 44]
  EpiModel   : 2.4.0 -> 2.5.0                       (update) [730, 44]
...
DiceDesign  : 1.10 Imports from dials              (add) [730, 126]
  sfd        : 0.1.0 Imports from dials            (add) [730, 128]
  dials      : 1.4.0 Imports from tune              (add) [730, 129]
  doFuture   : 1.0.2 Imports from tune              (add) [730, 131]
  GPfit      : 1.0-8 Imports from tune              (add) [730, 133]
sparsevctrs : 0.3.1 Imports from parsnip           (add) [730, 136]
  parsnip    : 1.3.1 Imports from tune              (add) [730, 137]
modelenv    : 0.2.0 Imports from workflows         (add) [730, 140]
  workflows  : 1.2.0 Imports from tune              (add) [730, 141]
  yardstick  : 1.3.2 Imports from tune              (add) [730, 143]
  tune       : 1.3.0 Imports from tidyposterior     (add) [730, 144]
workflowsets : 1.1.0 Imports from tidyposterior    (add) [730, 146]
  tidyposterior : 1.0.1                             (keep) [730, 146]
```



# BioInformatics Packages – Pyro-Velocity

## Pyro -Velocity

Probabilistic modeling of RNA velocity



## Pyro-Velocity

- 83 Dependencies listed in pyproject.toml
- Most dependencies are available with EB but not all in from the same toolbox
- Manual install does not pass pip check
- Documentation is incorrect – Examples do not work
- Hybrid EasyConfig with hand built pip install
- Lua module has 33 modules
- module list shows 192 loaded modules
- Install is not reproduceable from the EasyConfig

The user is happy



# Thank you

John Dey

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GitHub fizwit

# HPC @ Fred Hutch

Recently form Data Science Department

<https://Dasl.fredHutch.org>

Published Module List

<https://fredhutch.github.io/easybuild-life-sciences/>

HPC team members contribute one hour per week to support SciWiki Documentation

<https://SicWiki.FredHutch.org>