polars-bio: High-Performance Python DataFrame Operations for Genomics

Demystify AI & Data Management Series

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About me



- ► Assistant Professor^a at Warsaw University of Technology
- ➤ Chief Architect @Xebia Data Poland, 20+ years building data-intensive systems
- distributed and data-intensive systems, artificial intelligence and cloud computing for large scale genomic studies.
- ▶ road and gravel bikes enthusiast
- ► https://marekwiewiorka.org/

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Biodatageeks lab

- Warsaw University of Technology, Faculty of Electronics and Information Technology
- - ► AI for analyzing biomedical literature
 - Meta-calling for gene fusion detection in RNA-Seq
 - Optimizing RVAS
 - ▶ Open genomic data lakehouse
- https://biodatageeks.org/
- ► https://github.com/biodatageeks/

Meet the Team

Principal Investigators





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Researchers



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BSc Student



Ostrowska PhD student



Wojciech Sitek Research Assistant



Piotr Suszyński PhD student



Agnieszka Szmurło PhD Student

Agenda

- 1. Pationale and motivation
- 2. Kara Context and alternatives for polars-bio
- 3. 🔬 Deep dive into internals
- 4. Benchmarks
- 5. **§** Future directions

Introduction to polars-bio

- ▶ polars-bio is a novel Python DataFrame library for genomics that is *fast* and *memory-efficient*, introduced in 2025, built on top of Polars, Apache DataFusion and Apache Arrow.
- main focus areas:
 - ▶ 🔊 genomic interval operations
 - scalable data processing and querying
 - ▶ 💾 fast I/O for bioinformatics file formats
 - cloud storage interoperability
 - genomic data lakehouse readiness



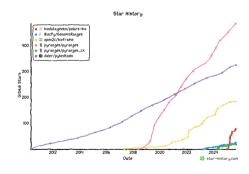
Rationale, History, and Challenges

- ► Growing bioinfo dataset sizes vs. increasing capacity of commodity hardware
- ► ★ Trade-off: scalability of distributed systems (e.g., Apache Spark Hail, Glow) vs. simplicity and performance of single-node libraries (e.g. DuckDB)
- ▶ Single-node solutions: constrained in both performance and scalability
- First attempt (2019–2023): SeQuiLa project on top of Apache Spark
- ► Conclusion: towards a *hybrid* approach



Landscape of tools for genomic interval operations in Python

- ▶ several widely used libraries exist in this space:
 - ▶ Pyranges and new Pyranges1
 - ► Pybedtools
 - **▶** Bioframe
 - ▶ GenomicRanges
- employing an eager, in-memory execution model with Pandas DataFrames/ NumPy arrays
- ► sweep-line (Bioframe, Pyranges1) or Nested Containment List (Pyranges, GenomicRanges) or genome binning algorithm (Pybetools)
- focus primarily on optimizing genomic operations rather than end-to-end processing and IO operations



Market trends in data systems

- ▶ out-of-core (streaming) processing
- ▶ single node vectorized engines e.g. DuckDB, Polars
- ▶ lazy evaluation and query optimization e.g. Polars
- open data standards and interoperability, such as Apache Arrow or Apache Iceberg
- composability and reusability, e.g. query parsers, optimizers, query engines, memory and file/table formats
- data lakehouse architecture









Composable Data Management Systems (CDMS) Manifesto

- ▶ **Problem**: Data systems are *fragmented*, *duplicated*, hard to maintain
- ▶ **Vision**: Break *monoliths* into *modular*, *reusable* components (frontends, Internal Representation, optimizers, execution engines, runtime environments)
- ▶ Why Now: Already existing *open standards* (Arrow, Parquet, Iceberg) enable composability
- ► Examples: Velox, Apache DataFusion
- ▶ **Benefits**: *Faster* innovation, *reduced* engineering effort, consistent user experience

Limitations of Current Approaches to Genomic Interval Processing

Genomic intervals processing is closer to BI/DWH/ETL-style workloads than to numerical computing!

- ► Relying on libraries (e.g., NumPy) not designed for efficient bioinformatics data handling
- ▶ Re-implementing algorithms and reinventing the wheel instead of leveraging mature *query engine*: optimizers, operators and open data standards
- ► Parallelism and out-of-core not treated as a first-class concern (limited scalability)
- ▶ *Naive* Python implementations (slow, limited scalability)
- ▶ Missing end-to-end optimization including reading, processing and writing data

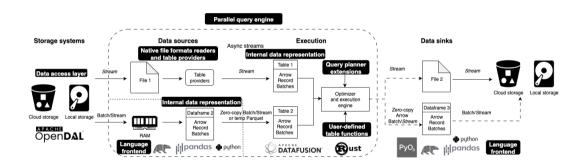
Why polars-bio is different?

- ► Composable and best of breed approach
 - query engine (Apache DataFusion)
 - ► DataFrame library (Polars)
 - columnar memory format (Apache Arrow)
 - ▶ data structure for interval intersection queries (COITrees and Superintervals)
 - ▶ bioinformatics file formats (noodles)
- ▶ Builtin *lazy*, *out-of-core* and *parallel* computational model
- ▶ IO layer optimizations for analytical queries, such as *projection* and *predicate* pushdowns

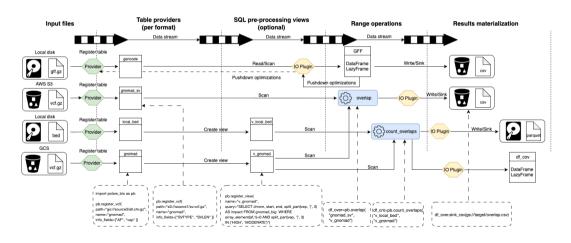


POLARS-BIO

polars-bio high-level architecture



Architecture deep-dive - core components



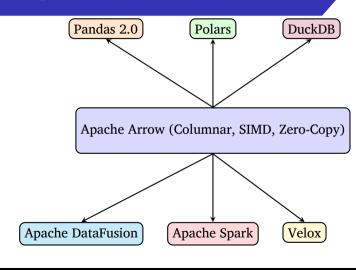
Architecture deep-dive - Polars and Apache DataFusion primer

- ► Polars and Apache DataFusion exhibit significant similarities, such as Apache Arrow columnar memory model, lazy evaluation and out-of-core computational model, great performance
- ▶ different main focuses:
 - ▶ Polars feature-rich end-user DataFrame library
 - ► DataFusion extremely extensible query engine for building custom data systems
- ▶ do we really need both?
 - ▶ Polars' great data wrangling capabilities but hard to extend
 - ▶ DataFusion's codebase reusability (e.g. hybrid execution) and more robust abstractions for query and IO optimizations
 - ▶ additional integration complexity (e.g. pushdown optimizations, parallelism control)



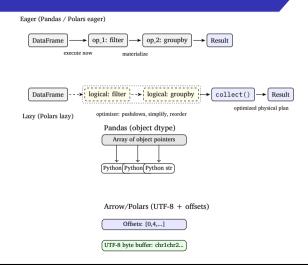
Architecture deep-dive - Apache Arrow

- Standardized columnar memory format – zero-copy sharing
- Vectorized execution: SIMD and CPU cache efficiency
- Cross-language interoperability (e.g. Python and Rust)
- ► Integration with open standards – Parquet, Iceberg
- ► Foundation for modern data systems – Polars, Ray, Rapids, Apache Spark



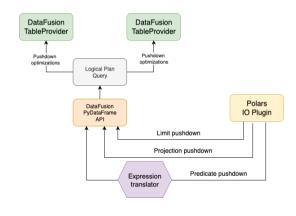
Architecture deep-dive - Polars vs. Pandas

- Execution model: Pandas is eager-only; Polars supports eager and lazy.
- Optimization: Pandas has no query optimizer;
 Polars (lazy) performs projection/predicate
 pushdown, simplification, reordering.
- ► Parallelism: Pandas mostly single-threaded (Python/GIL); Polars is multi-threaded (Rust).
- Memory/layout: Pandas uses NumPy blocks;
 Polars is columnar and Arrow-friendly.
- Out-of-core/streaming: Pandas primarily in-memory; Polars supports streaming/out-of-core in lazy plans.
- String handling: Pandas often stores Python objects (high memory overheads); Polars stores UTF-8 natively with efficient kernels (SIMD).



Architecture deep-dive - Polars IO plugin

- arbitrary function that returns a generator (Iterator) producing pl.DataFrame batches and gets back LazyFrame
- used for both files scanning and interval operations results streaming
- zero-copy and streaming using Arrow RecordBatchStream with DataFusion PyDataFrame
- support for limit, projection and predicate pushdowns (currently only GFF)



Architecture deep-dive - input file formats

- ► subproject datafusion-bio-formats
- ▶ exposed using custom TableProviders
- support for parralel reading of BGZF inputs
- ► local and cloud storage (AWS S3, GCS and Azure Blob
- cloud storage supported features

Format	Single- threaded	Parallel	Limit pushdown	Predicate pushdown	Projection pushdown
BED	✓	×	✓	×	×
VCF	✓	999	✓	999	999
ВАМ	~	×	✓	×	×
FASTQ	✓	V	✓	×	×
FASTA	~	×	✓	×	×
GFF3	V	✓	▽	V	V

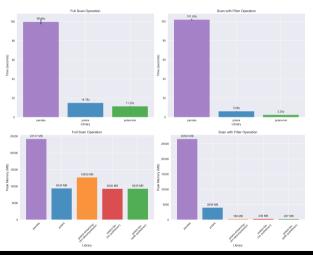
Benchmarking dataset

- AILIst real dataset converted into Parquet format – details
- ► GFF3 GENCODE release 49

Dataset#	Name	Size(x1000)	Description
Dataset#	Name	Size(x1000)	Description
0	chainRn4	2,351	Source
1	fBrain	199	Source
2	exons	439	Dataset used in the BEDTools tutorial.
3	chainOrnAna1	1,957	Source
4	chainVicPac2	7,684	Source
5	chainXenTro3Link	50,981	Source
6	chainMonDom5Link	128,187	Source
7	ex-anno	1,194	Dataset contains GenCode annotations with ~1.2 million lines, mixing all types of features.
8	ex-ma	9,945	Dataset contains ~10 million direct-RNA mappings.

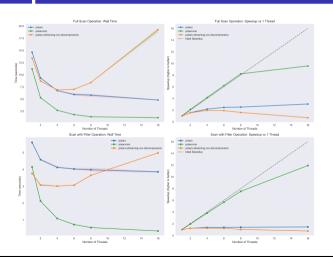
Source: Jianglin Feng, Aakrosh Ratan, Nathan C Sheffield, *Augmented Interval List:* a novel data structure for efficient genomic interval search, Bioinformatics 2019.

File formats: GFF (scan_csv vs polars-bio) – results 1/2



- ▶ in full-scans Polars and polars-bio significantly outperform Pandas
- ► Polars problem with scan_csv and compressed files)
- streaming decompression plugin

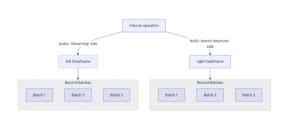
File formats: GFF (scan_csv vs polars-bio) – results 2/2



- polars-bio achieves near-linear scaling up to 8 threads
- ► Polars and streaming decompression plugin scale poorly

Architecture deep-dive – genomic interval operations 1/2

- ► inspired by the Hash Join implementation in DataFusion
- ► the *entire* (coordinates) build side is read into the interval search data structure
- batches from the probe side are streamed through and checked against the contents of the search data structure

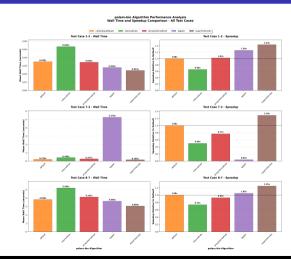


Architecture deep-dive – genomic interval operations 2/2

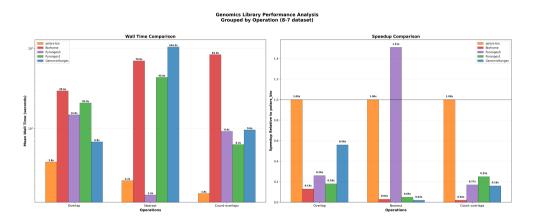
- ► subproject sequila-native
- ► custom PhysicalPlanner and PhysicalOptimizerRule for detecting and rewriting generic interval join operation (overlap or nearest)
- ► User-Defined Table Function (UDTF) for operations, such as coverage or count overlaps
- several data structures available:
 - ▶ COITrees
 - ▶ IITree
 - ► AVL-tree
 - ▶ rust-lapper
 - Superintervals

Genomic interval operations – structures comparison results 1/6

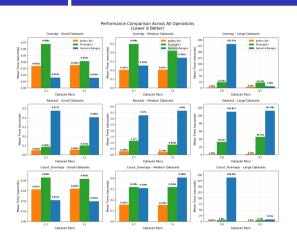
- ► COITrees (polars-bio default) and Superintervals fastest in all test cases
- configurable in runtime
- more tests using different datasets characteristics needed



Genomic interval operations – results 2/6

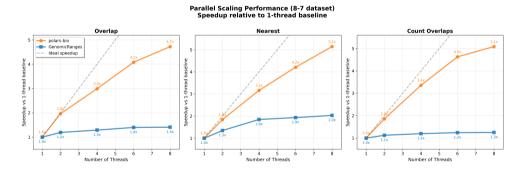


Genomic interval operations – results 3/6

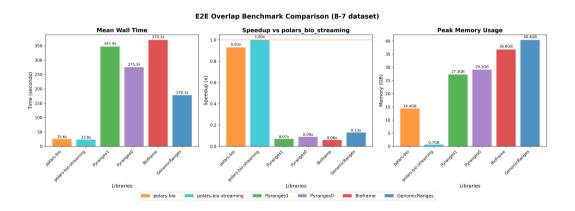




Genomic interval operations – scaling – results 4/6



Genomic interval operations – e2e pipeline – results 5/6



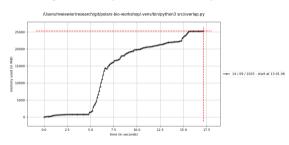
Genomic interval operations – results 6/6

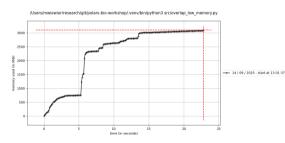
```
import pandas as pd
>> df = pd.read parquet("/tmp/exons/")
# GenomicRanges - int32
GenomicRanges(number of ranges=438694, segnames=[].
ranges=IRanges(
    start=array([], shape=(438694,), dtype=int32),
    width=array([], shape=(438694,), dtvpe=int32)).
# Bioframe - int32
cols=["contig","pos start","pos end"]
»> bf.from anv(df. cols=cols).info()
<class "pandas.core.frame.DataFrame'>
RangeIndex: 438694 entries, 0 to 438693
Data columns (total 3 columns):
     Column
               Non-Null Count
                                Dtupe
     contig 438694 non-null
                                 object
     pos start 438694 non-null
                                 int32
     pos end
               438694 non-null
                                int32
dtypes: int32(2), object(1)
```

```
# Puranaes0 - int64 !!!
»> df2pr0(df)
                 Start
                              End
  Chromosome
  (category)
                 (int64)
                              (int64)
                 11873
                              12227
  chr1
  chr1
                 12612
                              12721
  chr1
                 13220
                              14409
  chr1
                 14361
                              14829
Unstranded PyRanges object has 438.694 rows and 3 columns.
# Puranaes1 - int32
»> df2pr1(df)
index
                             Start
                                       End
              Chromosome
                             int32
                                       int32
int64
              object
              chr1
                             11873
              chr1
                            12612
              chr1
                            13220
                                       14409
              chr1
                             14361
                                       14829
PyRanges with 438694 rows, 3 columns, and 1 index columns.
```

Overlap operation low memory mode for $\sim 10^9$ wide rows

Capped (max rows per batch) streaming-friendly emission $-\sim 30-50\%$ slower but with significantly lower memory utilization.





polars-bio roadmap

- ▶ **Lakehouse support with open standards**
- ▶ 💾 Feature parity across all supported bioinformatics formats
- ▶ 📝 Write-back into table formats (e.g. Apache Iceberg)
- ▶ ia Spec-driven agentic development for automated pipelines
- ▶ 🚀 Hybrid execution: SeQuiLa + Apache Comet accelerator
- ► ≯ Your use case!

Summary

- ▶ 🔊 polars-bio: a new Python DataFrame library for genomics
- Combines Polars, Apache DataFusion, and Apache Arrow for speed and scalability
- ▶ 💾 Efficient I/O for popular bioinformatics formats
- ▶ ﷺ Addresses limitations of existing interval processing tools
- ▶ ¶ Towards a hybrid, lakehouse-ready approach for large-scale genomics

Stay Tuned!

- ▶ **♦** Project page: biodatageeks.org/polars-bio
- ▶ ¶ Meet us at ASHG 2025 Annual Meeting, Boston, October 14-18, 2025

Thank You!





Questions

Hands-on Demo



github.com/biodatageeks/polars-bio-workshop