Characterizing Large Applications Through Proxy Benchmarks: a Pangenomic Case Study

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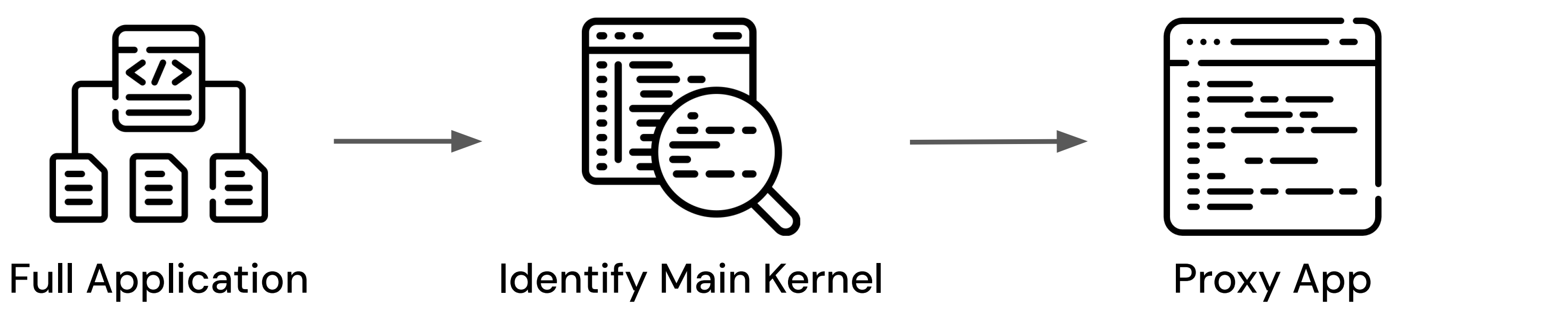
Introduction

- Large scientific applications are difficult to benchmark
- Involve complex inputs and many dependencies
- Can be inflexible to port to new hardware
- As a consequence, can be hard to be improved

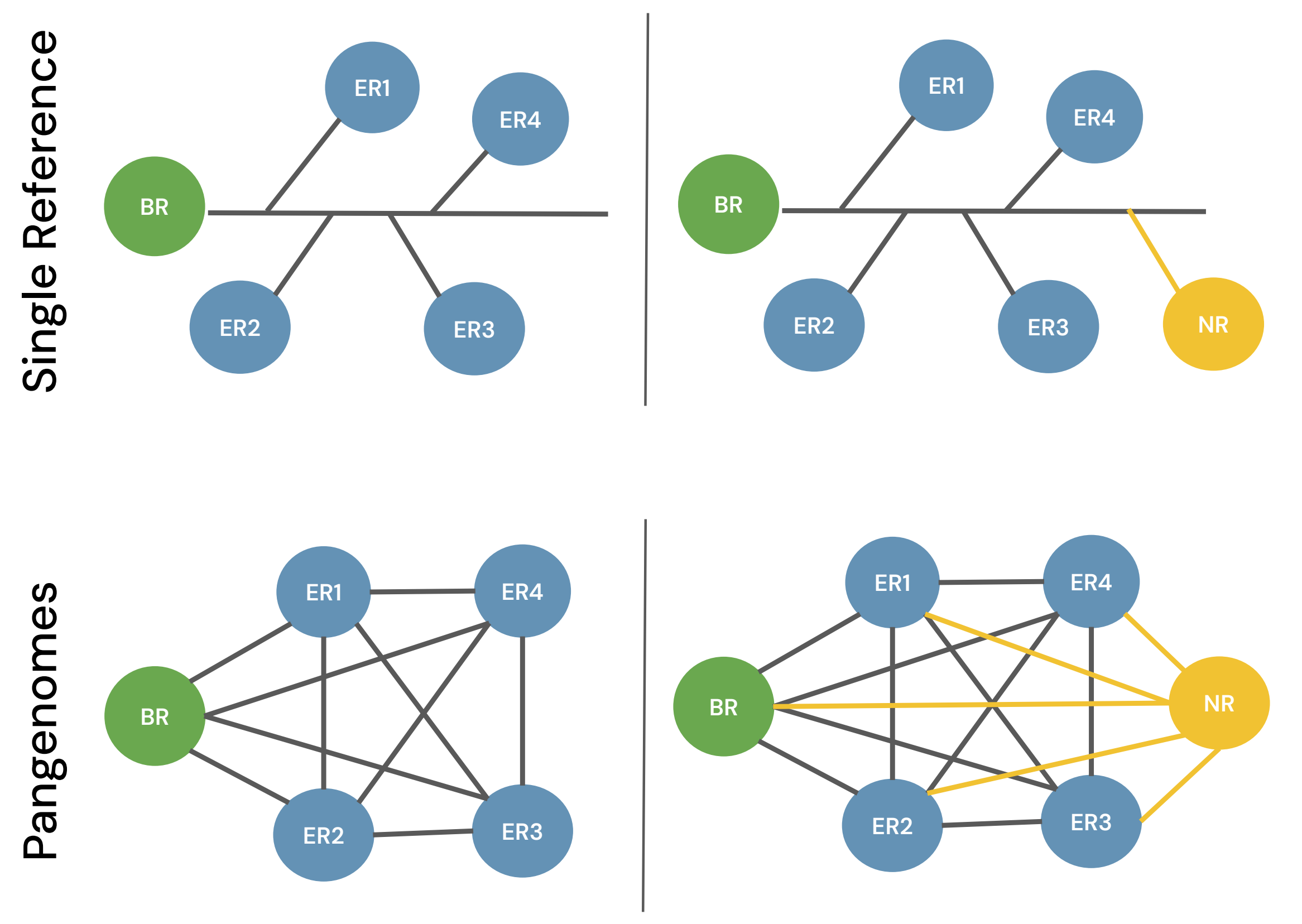
Proxy Apps can be a **lightweight** representation of real workloads that **ease performance** and **portability exploration**



In this work, we take the first steps to create a proxy application from an emerging and complex pangenomic application that maps short-read genomes to a pangenome graph reference.

Pangenomes

- Collection of common and unique genomes that are present in a given species [1]
- Composed of sequences from different individuals
- A more complete representation of a species' genome
- Complex DNA graph-based structure
  - Complexity to map sequences to this reference

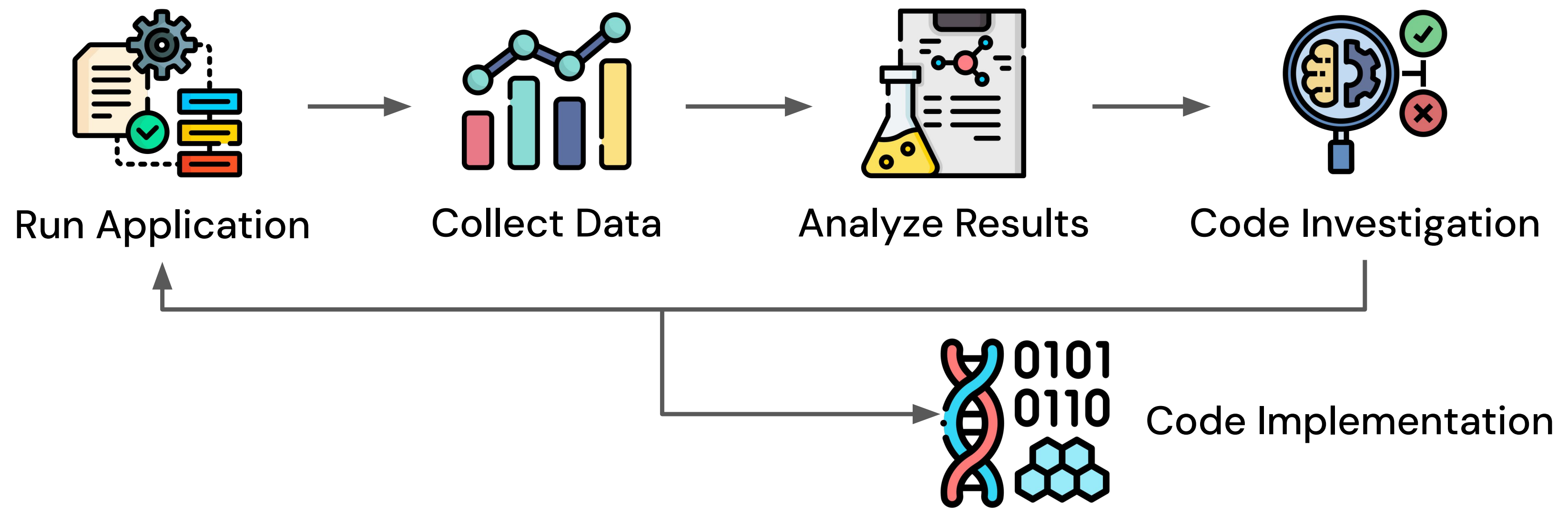


Single Genomes can be augmented with variations but do not contain all possible cross-references

Pangenomes allow to relate all genomes or sequences directly to each other

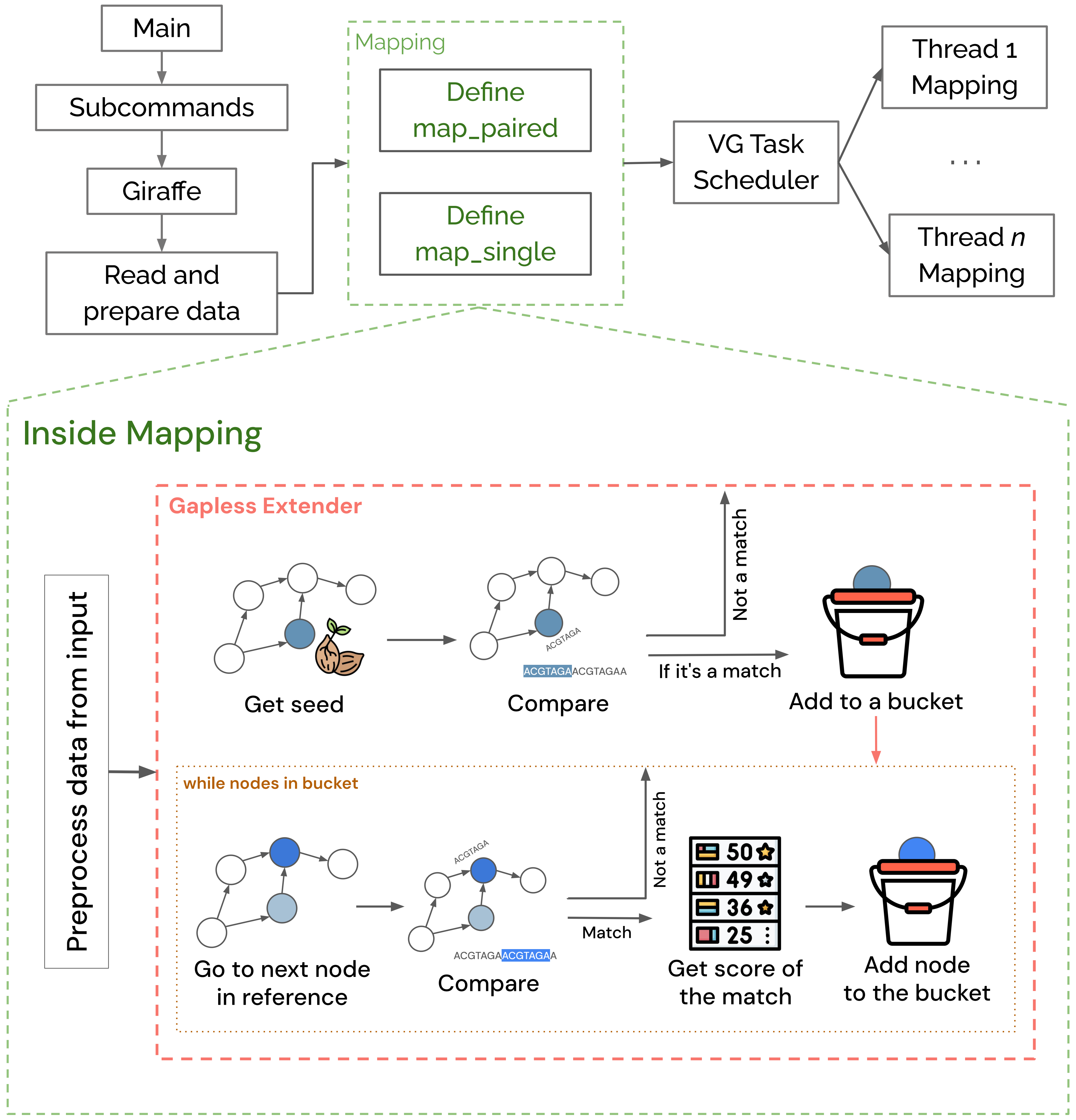
Source: Practical Graphical Pangenomics [https://pangenome.github.io/]

Proxy Generation Methodology



Pangenome Mapping Tool

We base our proxy app efforts on the *Giraffe* pangenome mapping tool [2]. Giraffe is one of the tools present in the *VG Toolkit* [3], which is a collection of tools focused on the creation and mapping of genome references as Variation Graphs



VG x Proxy

VG

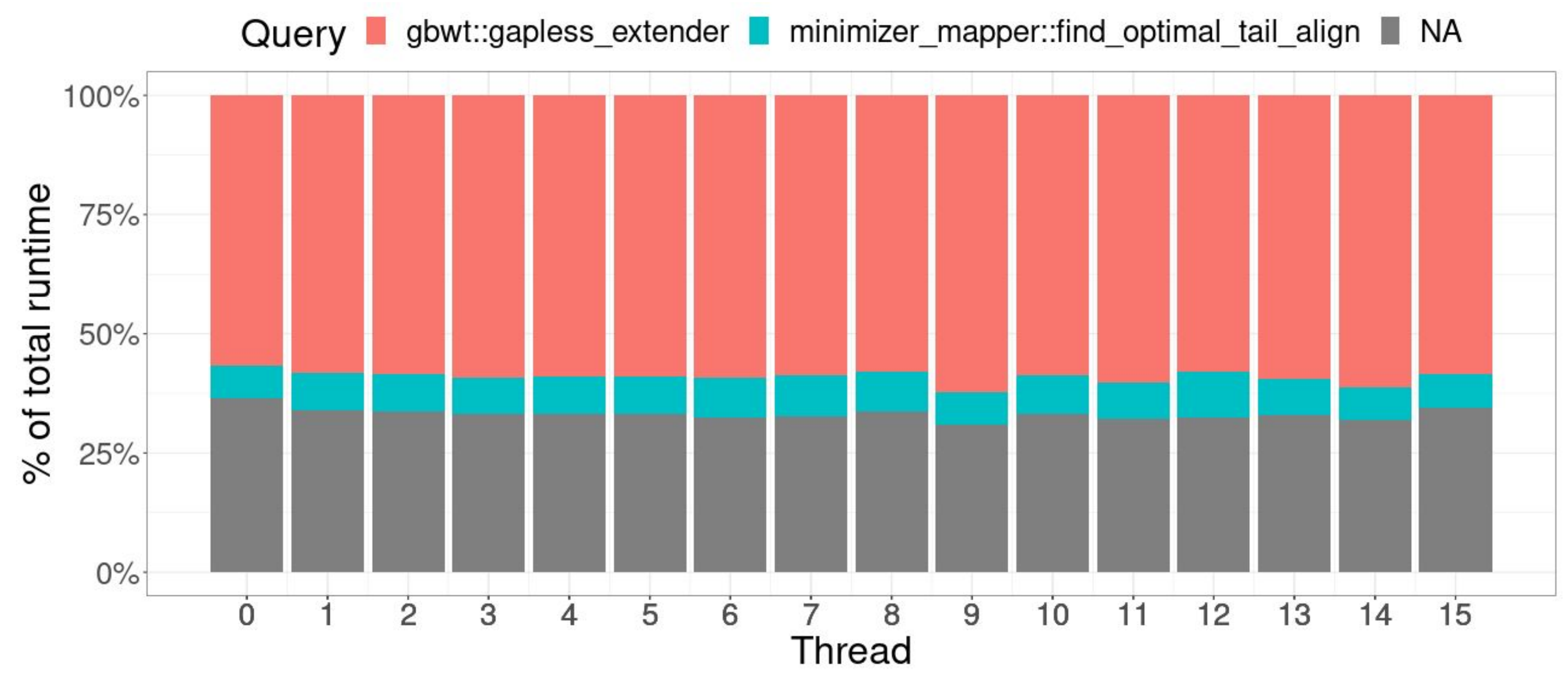
- ~50k lines of code
- ~350 source-files
- ~50 library dependencies
- Complex Makefile to compile
- More than 60s to compile
- Hard to profile

Proxy

- ~1k lines of code
- 2 source-files
- 3 library dependencies
- Simple Makefile to compile
- Around 10s to compile
- Easy to profile and play with different strategies

Profiling Results

To identify the most important mapping code within Giraffe, we profile the two functions that access the pangenome graph: the *gapless_extension* function and the *find_optimal_tail_alignment* function. *gapless_extender* represents more than 60% of the application's runtime in all threads.



[1] Abondio P, Cilli E, Luiselli D. Human Pangenomics: Promises and Challenges of a Distributed Genomic Reference. Life (Basel). 2023 Jun 9;13(6):1360. doi: 10.3390/life13061360. PMID: 37374141; PMCID: PMC10304804.
[2] Jouni Sirén et al. ,Pangenomics enables genotyping of known structural variants in 5202 diverse genomes.Science374,abg8871(2021).DOI:10.1126/science.abg8871
[3] Garrison, E., Sirén, J., Novak, A. et al. Variation graph toolkit improves read mapping by representing genetic variation in the reference. Nat Biotechnol 36, 875–879 (2018). https://doi.org/10.1038/nbt.4227
[4] Cook, Jeanine, Finkel, Hal, Junghams, Christoph, McCorquodale, Peter, Pavel, Robert, & Richards, David F. Proxy App Prospectus for ECP Application Development Projects. United States. https://doi.org/10.2172/1477829

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