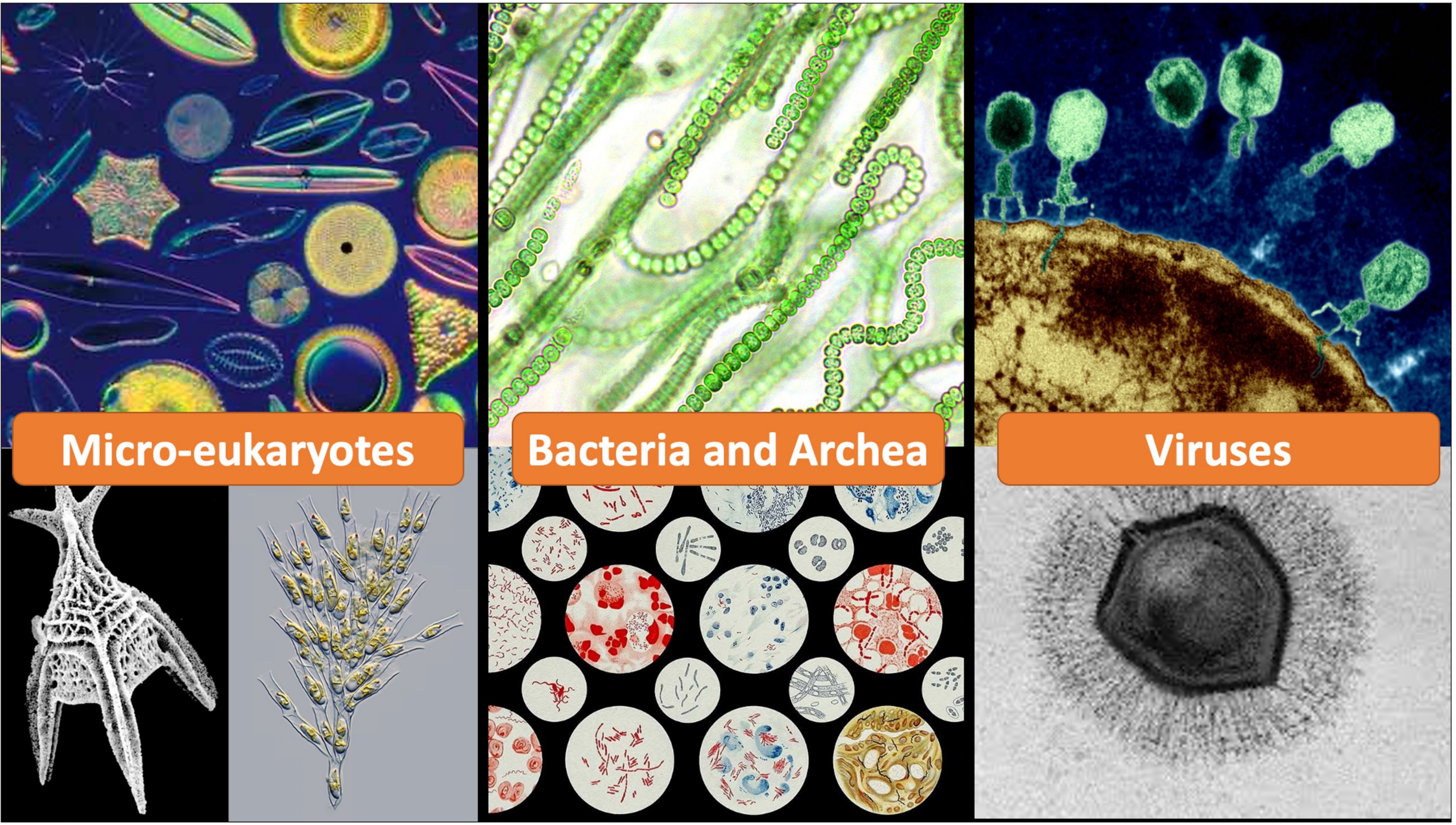
Hewlett Packard
Enterprise

Exploring Suffix Array Algorithms in Chapel

Michael P. Ferguson, Bonnie Hurwitz, Shreyas Khandekar

PAW-ATM 2024
November 17, 2024

What is a microbiome?



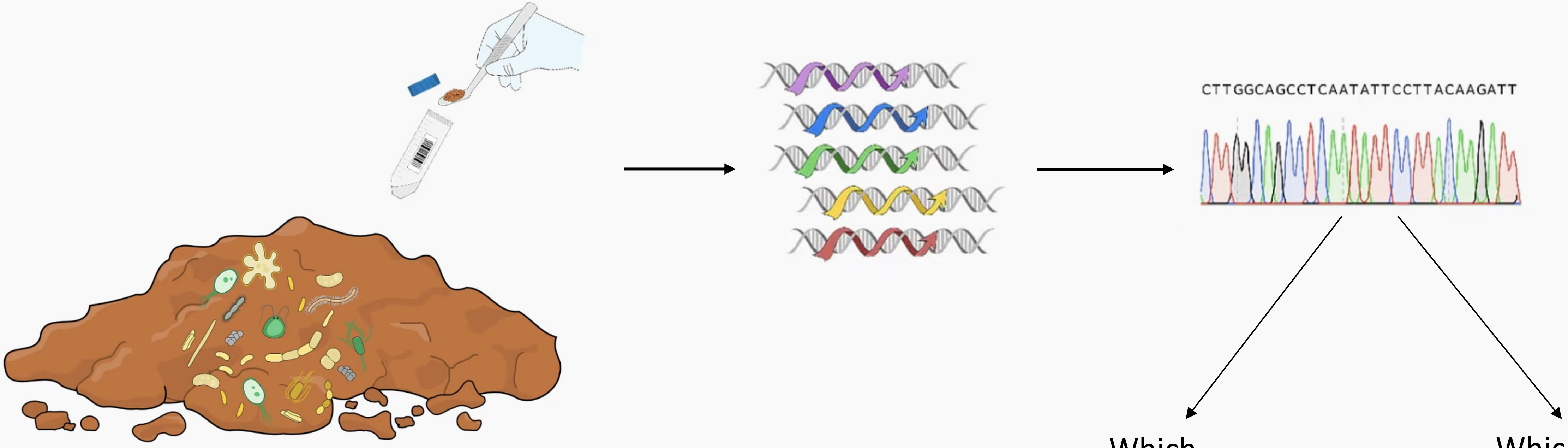
A **microbiome** is a complex mixture of microorganisms that reside in a specific environmental niche.

OHMI: https://doi.org/10.1186/s13326-019-0217-1

@thescientist

The human microbiome is an essential organ whose functions are central to human health

Microbial metagenomics allows us to explore the complex interaction between microbiota and host health



Which bacterial species?

Which bacterial strains?

Metagenomics is the genomic analysis of microbial communities by extracting and sequencing their DNA. Metagenomics allows to study complex communities of microorganisms directly in their natural environment

Computational Approach

- Gather lots of genomes for known bacteria

- Analyze these genomes to find k-mers that identify a particular microbial strain
  - A k-mer is just snippet of the DNA sequence of length k; e.g. ACGTTATA is an 8-mer
  - An identifying k-mer should ideally only be present in the genome of a single microbial strain

Focus of this talk

- Search for these identifying k-mers within metagenomic samples to learn about microbial communities

Suffix Array

- Suffix Arrays are used in several bioinformatics applications including bowtie2 and MUMmer4 [1,2]
- We are exploring how suffix arrays can help to identify subsequences for strain-level detection
- What is a suffix array?

Suffixes of ‘seeresses’

Suffix	Offset
`seeresses`	0
`eeresses`	1
`eresses`	2
`resses`	3
`esses`	4
`sses`	5
`ses`	6
`es`	7
`s`	8

Sorted Suffixes

Suffix	Offset
`eeresses`	1
`eresses`	2
`es`	7
`esses`	4
`resses`	3
`s`	8
`seeresses`	0
`ses`	6
`sses`	5

The Suffix Array

The Chapel Parallel Programming Language

Chapel is a language designed for productive parallel programming, particularly on large-scale systems. Chapel is …

Easy to Use	"*We ask students at the master's degree to do stuff that would take 2 years and they do it in 3 months.*" Eric Laurendeau, Professor of Mechanical Engineering
Portable	HPE Cray EX, HPE Apollo, Cray XC, *nix systems, Mac, NVIDIA and AMD GPUs
Fast & Scalable	Achieved 8,500 GiB/s when sorting 256 TiB in 31 seconds on 8192 HPE Cray EX Nodes
GPU-Ready	Real-world applications were ported on GPUs with few changes, and run on leadership-class systems such as Frontier and Perlmutter
Open source	Team at HPE actively interacts with Chapel community at chapel-lang.org

What did we do?

- We implemented several tools to explore how suffix arrays can be applied to strain detection

- Suffix Array Construction in Chapel
  - Implemented the Difference Cover algorithm [3] focusing on v=133
  - Also implemented parallel sparse PLCP array construction [4,5]

- Computing Similarity based on the Suffix Array
  - Use case: detect reference genomes that are too related to be useful for strain identification
  - Explored & implemented several parallel algorithms to compute all-to-all similarity for a set of genomes

- Finding Unique Substrings based on the Suffix Array
  - Use case: finding identifying k-mers for strain-level detection
  - Implemented a parallel algorithm to find all substrings that appear in just one genome [6]
  - If no unique substrings can be found for a genome, uses similarity computation to drop near-duplicate genomes

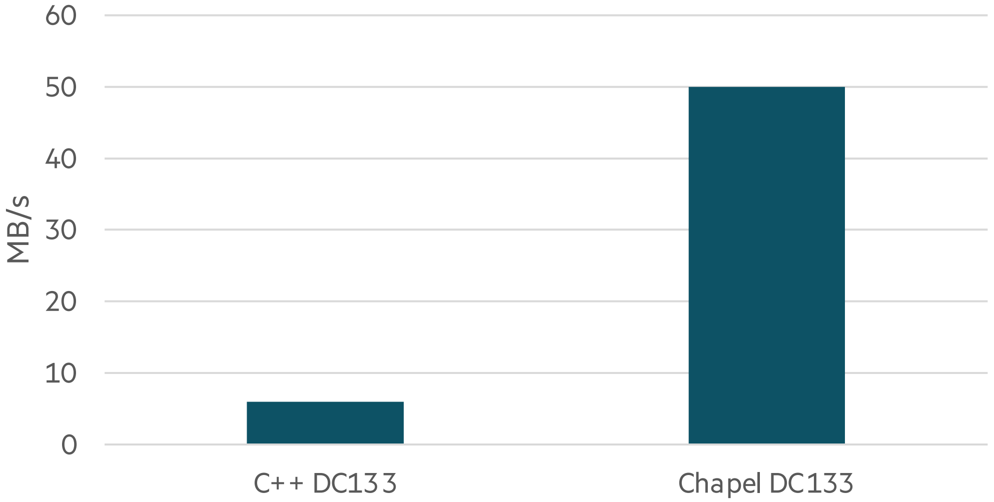
Experience Report: Productivity

- We were able to implement all 3 tools in less than a month
- We can compare the suffix array construction code against an earlier C++ implementation [7]
- Chapel version is about 2000 lines while the C++ implementation is closer to 8000 lines
  - Both implement the Difference Cover algorithm & have the same primary author
  - C++ implementation was parallel with MPI + OpenMP & optionally an external memory algorithm
  - The Chapel version is parallel and distributed (in-memory only)
  - Improvements are needed in both cases to achieve good scaling in distributed memory
- Challenges:
  - hit occasional minor bugs
  - tricky to identify and fix problems with distributed memory performance
- Benefits:
  - High level parallel loops with ‘forall’ help with straightforward and portable code
  - Generic programming to make it easier to implement
    - Difference covers that are compiled in based on ‘param’
    - When switching some arrays to be distributed, existing functions can accept & work with the distributed arrays

Experience Report: Performance of the Suffix Array Construction

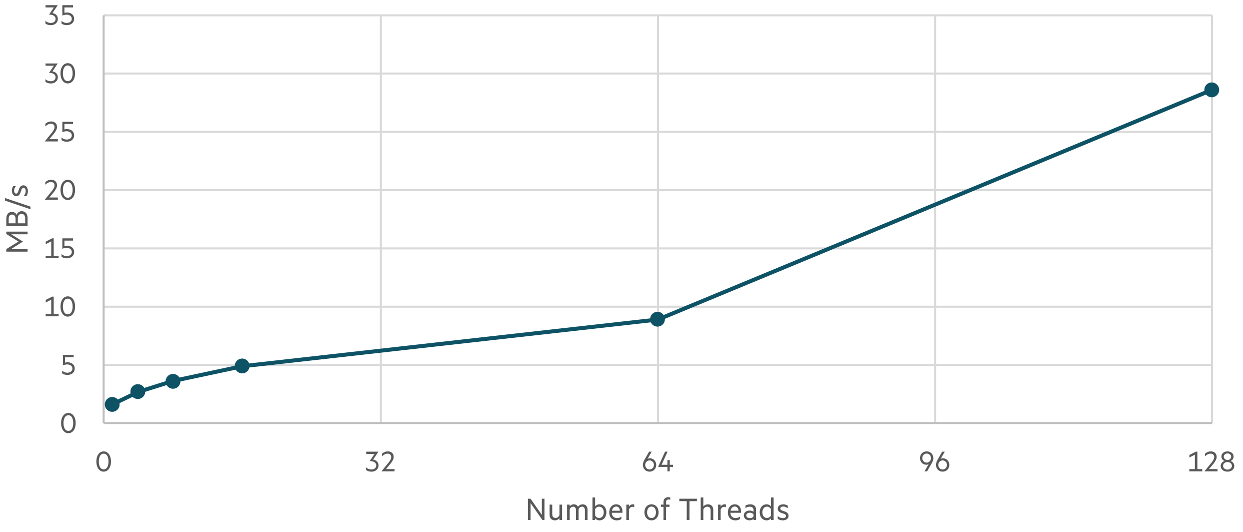
This chart compares the performance of the C++ and Chapel versions running in-memory on a single node

- On AMD Ryzen 9 7950X, 32 threads
- The C++ in-memory version is mostly serial
- Chapel version is parallel throughout



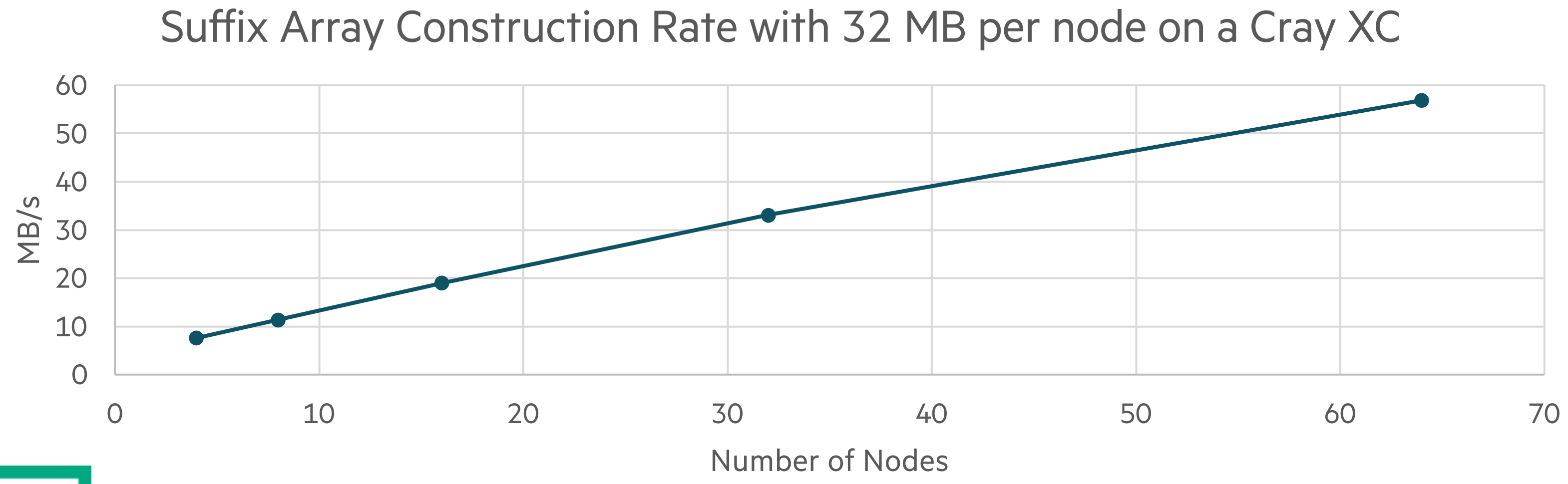
This chart shows single-node strong scaling

- On AMD EPYC 7543P 32-core processor
- Memory-intensive & can hit memory bottlenecks



Experience Report: Distributed Performance of the Suffix Array Construction

- Spent only a week making suffix array construction run multi-node
- Starting to use distributed arrays and run distributed was easy
- Trickier part was to identify and resolve performance issues
- Found the ‘local’ block in Chapel useful for identifying unexpected communication
  - Needed to arrange to do communication in a separate region for this strategy to work
- Achieved some scalability for a version with minimal random access (similar to external memory version)
  - This version is slower single-node & more memory intensive but reduces communication multi-node
  - Need both algorithmic improvements & implementation tuning to do better



Conclusion and Future Work

- This talk has shown some early results from our efforts
- We are using Chapel to implement tools to support strain-level metagenomic analysis

- We feel that Chapel has been particularly useful
  - for algorithmic exploration
  - to easily write parallel code
  - to easily move to distributed memory

- Scalable distributed-memory suffix array construction needs more work

- We are working towards publishing about our new tools in a bioinformatics journal

- Code is open-source & available at https://github.com/femto-dev/femto/tree/main/src/ssort_chpl

References

[1] B. Langmead, S. Salzberg, “Fast gapped-read alignment with Bowtie 2,” in *Nat Methods* vol 9, pp 357–359, 2012, doi: 10.1038/nmeth.1923

[2] G. Marçais, A. L. Delcher, A. M. Phillippy, R. Coston, S. L. Salzberg, and A. Zimin, “MUMmer4: a fast and versatile genome alignment system,” in *PLoS computational biology*, vol 14 no 1, 2018

[3] J. Kärkkäinen, P. Sanders, and S. Burkhardt, “Linear work suffix array construction,” in J. ACM vol. 53, no. 6, pp 918–936, Nov. 2006, doi: 10.1145/1217856.1217858

[4] J. Shun, "Fast parallel computation of longest common prefixes," SC '14: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, New Orleans, LA, USA, 2014, pp. 387-398, doi: 10.1109/SC.2014.37

[5] Juha Kärkkäinen, Giovanni Manzini, and Simon J. Puglisi. 2009. Permuted Longest-Common-Prefix Array. In Proceedings of the 20th Annual Symposium on Combinatorial Pattern Matching - Volume 5577. Springer-Verlag, Berlin, Heidelberg, 181–192.

[6] L. Ilie and W. F. Smyth, “Minimum unique substrings and maximum repeats,” in Fundam. Inf., vol 110, pp. 183-195, January 2011

[7] M. P. Ferguson, “FEMTO: fast search of large sequence collections,” CPM 2012: Combinatorial Pattern Matching 2012, in Lecture Notes in Computer Science, vol 7354, doi: 10.1007/978-3-642-31265-6_17 . Implementation available at https://github.com/femto-dev/femto/