Memory Efficient Minimum Substring Partitioning

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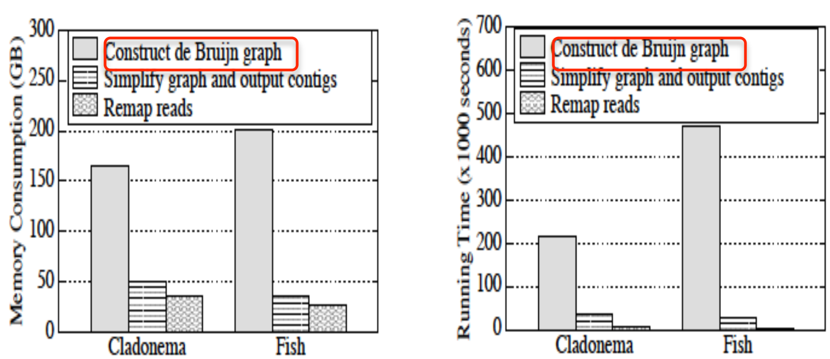
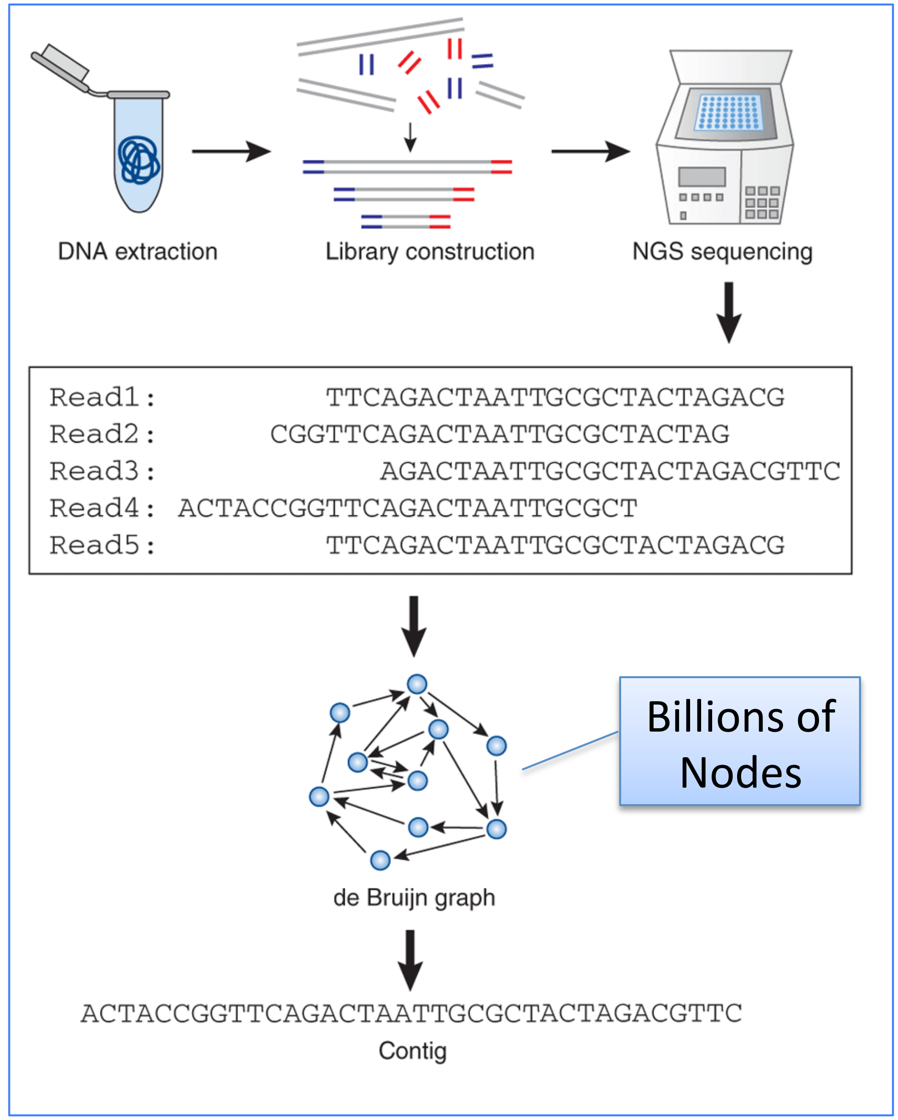
Motivation - Challenges

- De Bruijn graph based sequence assembly
- Building de Bruijn graph is both time intensive and memory consuming

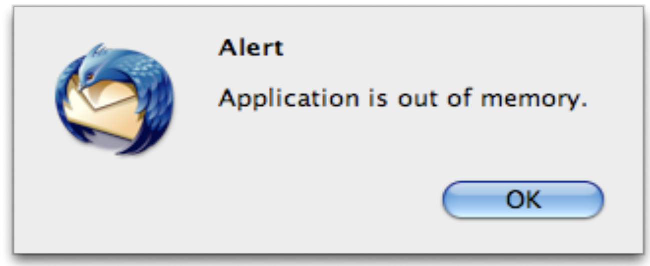


(a) *Peak Memory* (b) *Running Time*



Motivation - Existing solutions

- In-memory solution
  - 😊 Small running time
  - ☹ Huge memory footprint



- Classic disk-based approach
  - 😊 Small memory footprint
  - ☹ Huge disk space consumption
  - ☹ Very large running time

Objectives

- De Bruijn graph construction
  - ☺ with small running time
  - ☺ with small memory footprint
  - ☺ with small disk space consumption

- Minimum Substring Partitioning

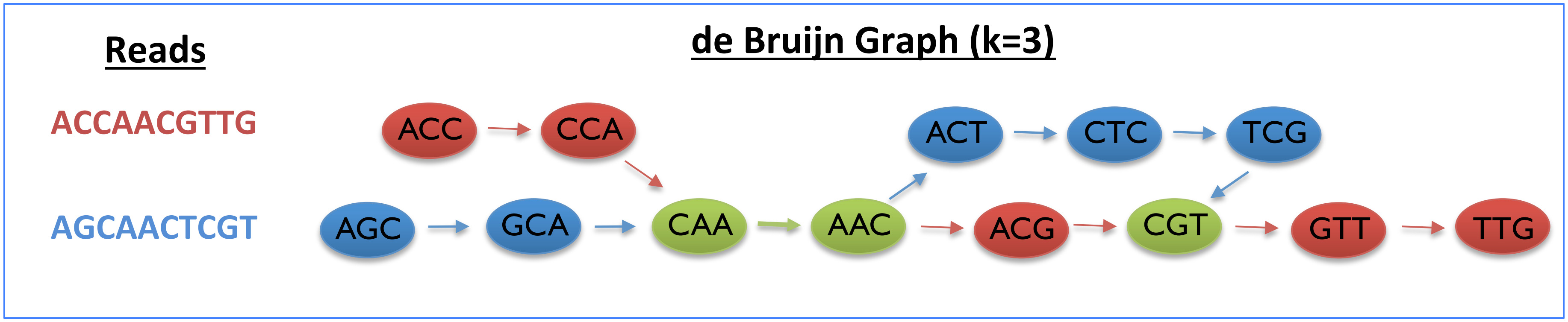
A disk-based method with a SMART partitioning strategy ☺

Outline

- Backgrounds
- Minimum Substring Partitioning (MSP)
- MSP-based de Bruijn graph construction
- Experiments
- Conclusions

Backgrounds - de Bruijn graph

- De Bruijn graph
  - G_k = (V,E)
  - V = All unique *k-mers* (length-k substrings)
  - E = Directed edges between consecutive k-mers
    - consecutive k-mers overlap by k-1 symbols
  - Human genome: >3B nodes, >10B edges



Backgrounds - Classic partitioning methods (1)

- Goal: deduplicate k-mers

- Horizontal Partition (***H-Partition***)
  1. partition reads S horizontally into disjoint subsets S_i
  2. for each S_i, build a hash table H_i of k-mers in memory
  3. output a sorted copy H_i to disk
  4. merge all such sorted hash tables

Pro: partitioning is simple and straightforward

Con: merging is very expensive (time consuming)

- same k-mer may appear in different partitions

Backgrounds - Classic partitioning methods (2)

- Goal: deduplicate k-mers

- Bucket Partition (***B-Partition***)
  1. partition(hash) all k-mers from S into disjoint subsets K_i
  2. for each K_i, build a hash table H_i of k-mers in memory
  3. output H_i (no need to sort) to disk
  4. merge all such hash tables

Pro: merging is simple and straightforward

Con: partitioning is very expensive (time consuming)

- k-mer set size is much larger than sequence set size
- huge I/O costs and disk space occupations

Minimum Substring Partitioning

Intuition

- if several adjacent k-mers are distributed to the same partition, we can compress them to reduce I/O costs

➕

Observation

- since two adjacent k-mers overlap with length k-1 substring, the chance for them to have the same minimum p-substring ($p < k$) could be very high.

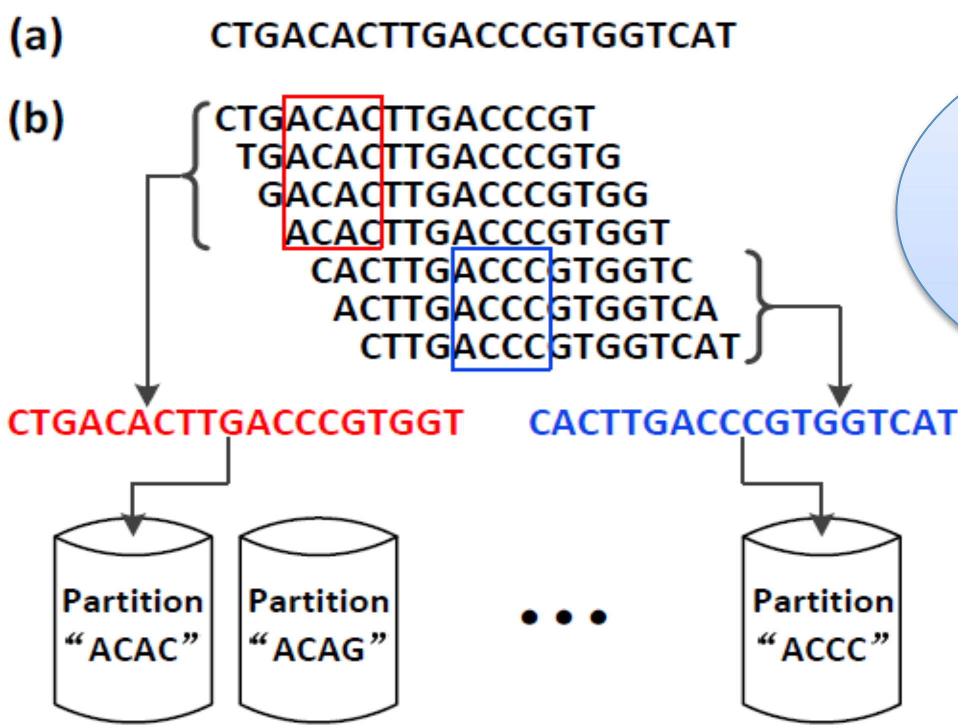
⬇

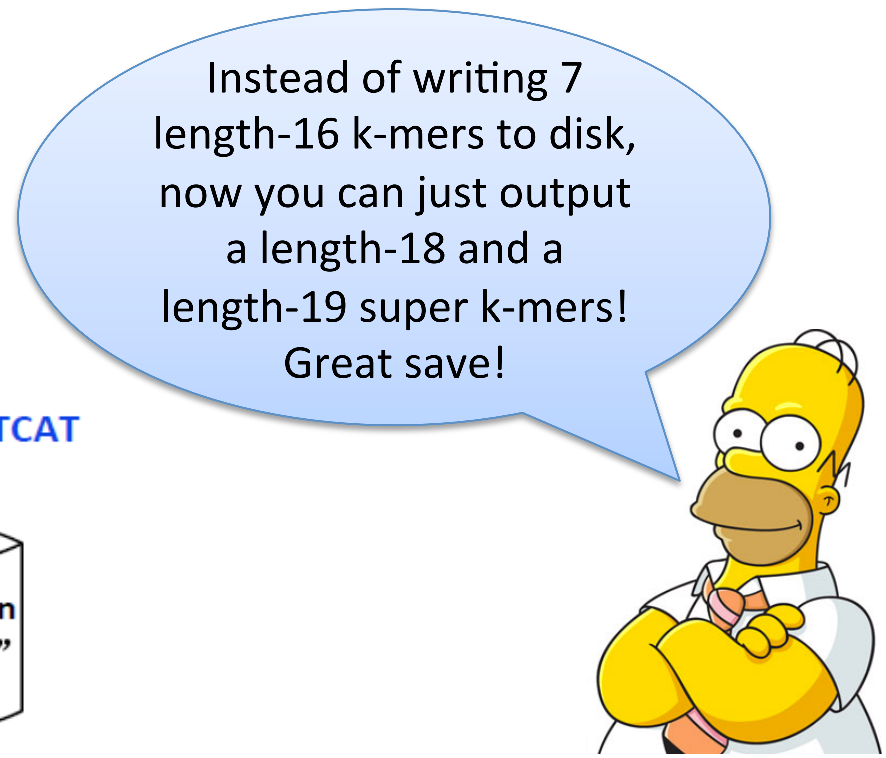
Idea

- partition k-mers w.r.t minimum substring

Minimum Substring Partitioning

Given a string $s = s_1 s_2 \ldots s_m$, $p \le k \le m$, *minimum substring partitioning breaks* s *to substrings with maximum length* $\{s[i,j] \mid i+k-1 \le j, 1 \le i, j \le m\}$, *s.t., all* k*-mers in* $s[i,j]$ *share the same minimum* p*-substring.* $s[i,j]$ *is also called super* k*-mer.*





Minimum Substring Partitioning - Theorems

- We employ a *random string model* to derive theorems
- Total Partition Size — critical for running time & disk space usage

Theorem 1

In a random string model, the total partition size is $O(pn)$ or $\Theta(n)$

- Largest Partition Capacity — critical for peak memory

Theorem 2

In a random string model, the maximum percentage of distinct k-mers covered by one p-substring is bounded by $3k/(4^p+1)$, when $p \geq 2$.

MSP-based de Bruijn graph construction

Partitioning

A simple yet efficient scan algorithm for MSP

↓

Mapping

Assign ID to each k-mer and generate ID replacement tables

↓

Merging

Merge ID replacement tables to produce a disk-based de Bruijn graph

Experiments - Setup

- Datasets

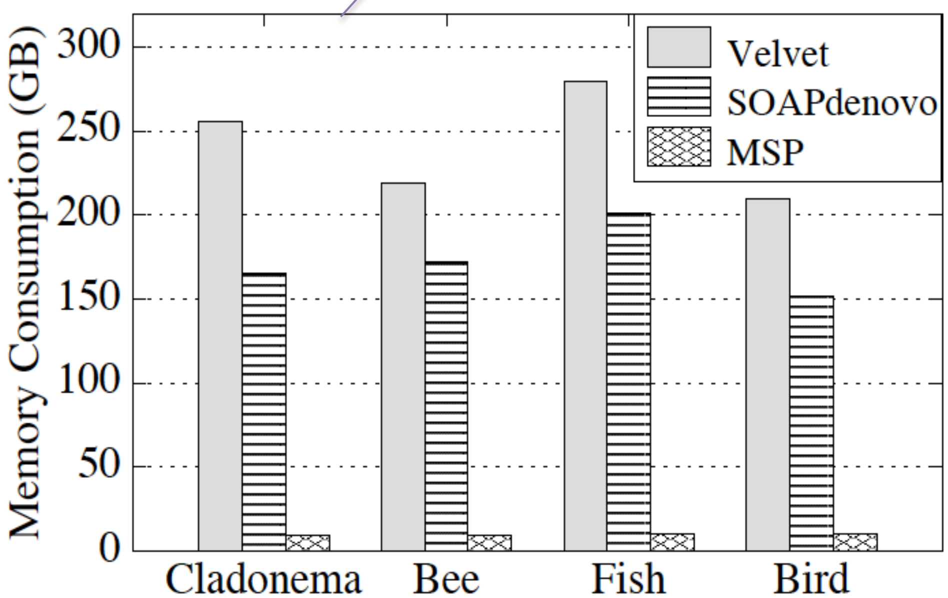
	Cladonema	Bee	Fish	Bird
Size (GB)	258.7	93.8	137.5	106.8
Avg Read Length (bp)	101	124	101	150
# of Reads (million)	894	303	598	323

- Environment
  - a server with 2.40GHz Intel Xeon CPU and 512GB RAM
- Evaluation criteria
  - Peak memory
  - Running time
  - Disk space usage

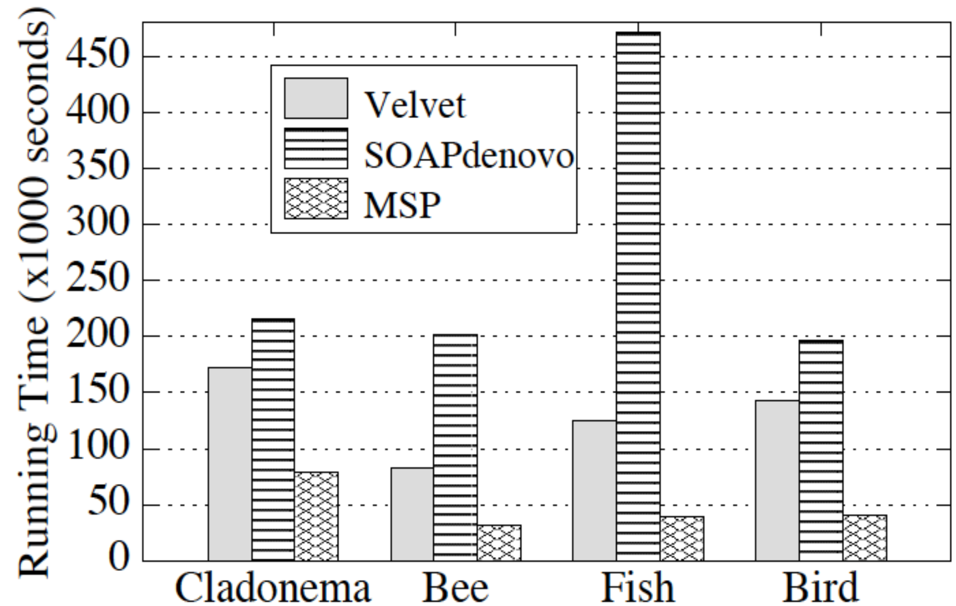
The smaller, the better!

Experiments - Efficiency

An order of magnitude reduction of memory usage

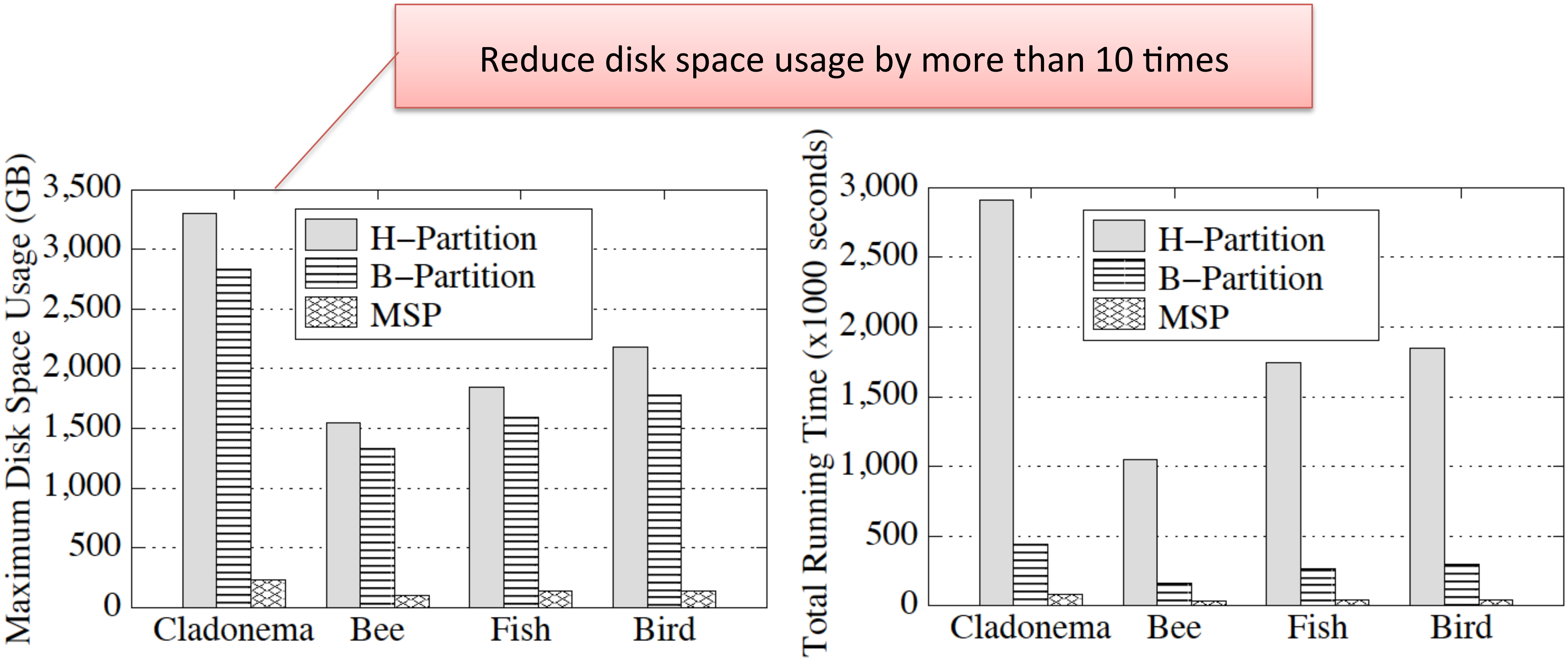


(a) *Peak Memory*



(b) *Running Time*

Experiments - Effectiveness

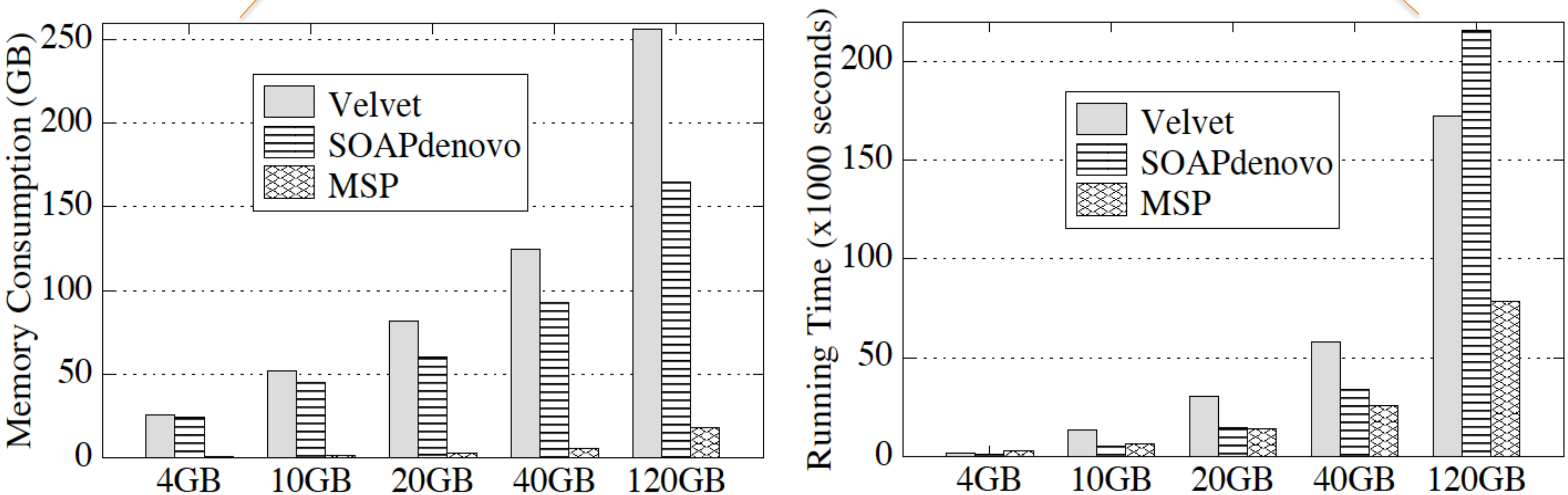


(a) *Max Disk Space Usage*

(b) *Running Time*

Experiments - Scalability

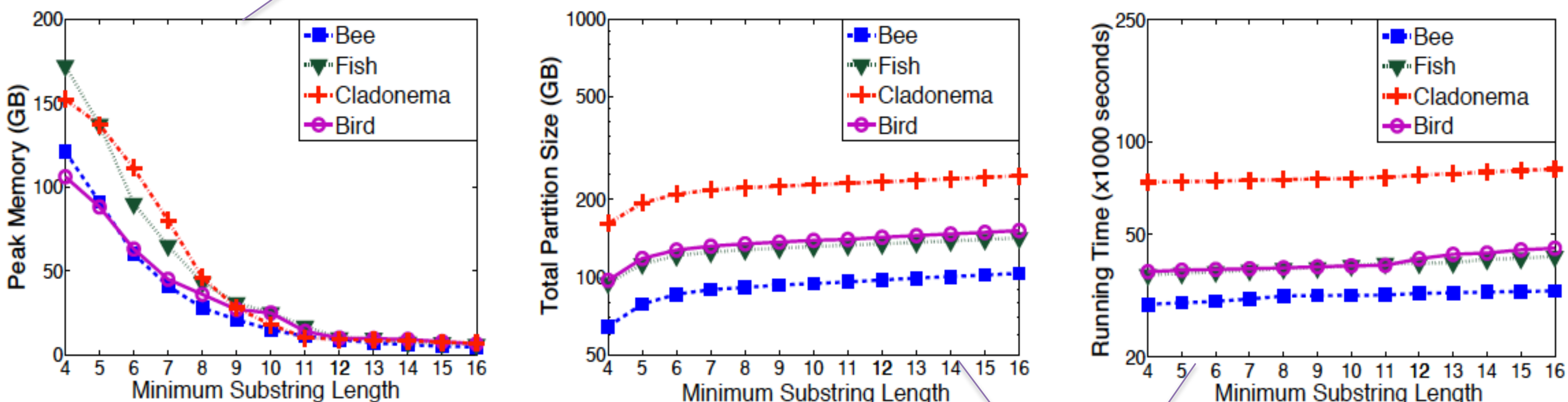
Linear scalability



(a) *Peak Memory* (b) *Running Time*

Experiments - Properties (1)

Peak memory decreases significantly as *p* increases

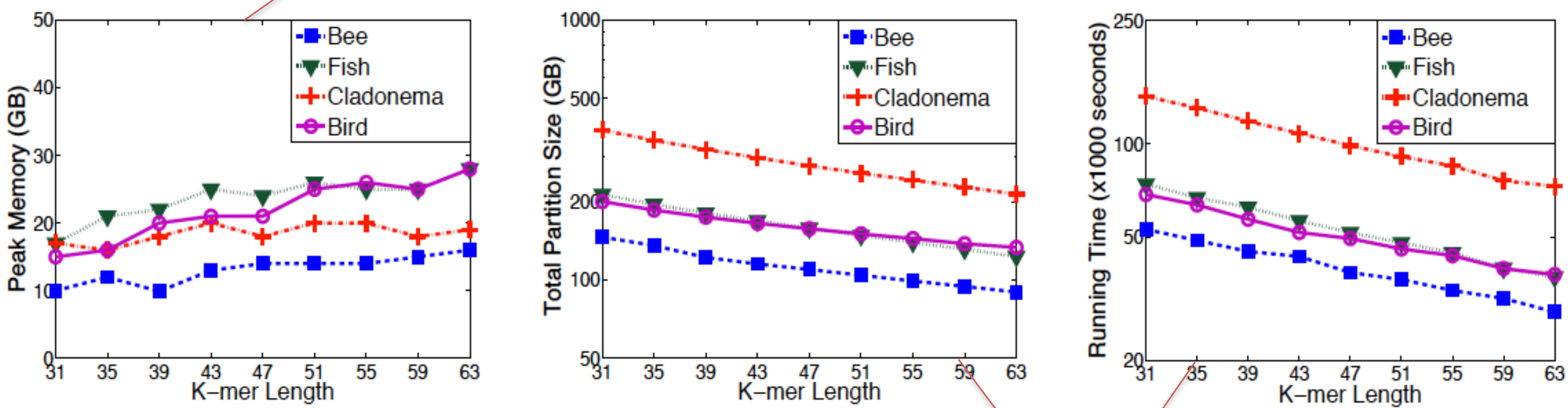


(a) *Peak Memory* (b) *Total Partition Size* (c) *Running Time*

Partition size and running time slightly increase as *p* increases

Experiments - Properties (2)

Peak memory increases slowly as *k* increases



(a) *Peak Memory* (b) *Total Partition Size* (c) *Running Time*

Partition size and running time decrease as *k* increases

Conclusions

- Minimum Substring Partitioning
  - with small running time
  - with small memory footprint
  - with small disk space consumption
- Project Homepage
  - *http://grafia.cs.ucsb.edu/msp*

Remaining Challenges

Sequence Assembly

- Construct de Bruijn graph

- Load graph & generate sequence


Thanks!