Hybrid parallel computing applied to DNA processing

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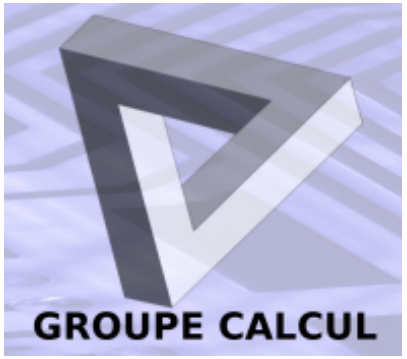


Outline

Genomics and New Generation Sequencing

Genomics

Genomics: studying the *Genome* of organisms.
Sequencing: extracting DNA text representation from cells.

New Generation Sequencing (NGS)

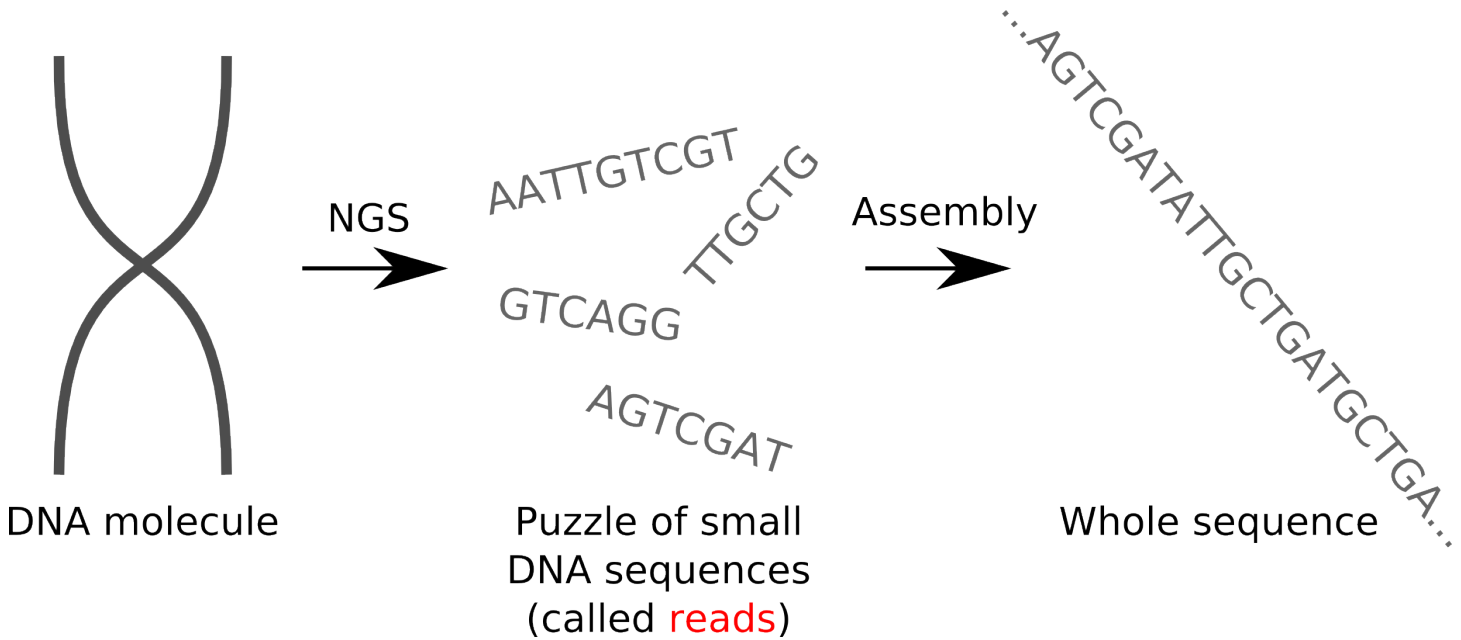
A recent breakthrough.
Faster sequencing. Produces huge amounts of raw data
(up to several gigabytes of text per use)

NGS-produced data must be processed
using text processing algorithms.
Amount of data $\Longrightarrow$ Long processing time with existing
sequential algorithms.

DNA assembly: a puzzle game

DNA sequence

A DNA sequence is a string on alphabet A, T, G, C.
A single letter from a DNA sequence is called a base.



Breaking reads into k-mers: De Bruijn graphs

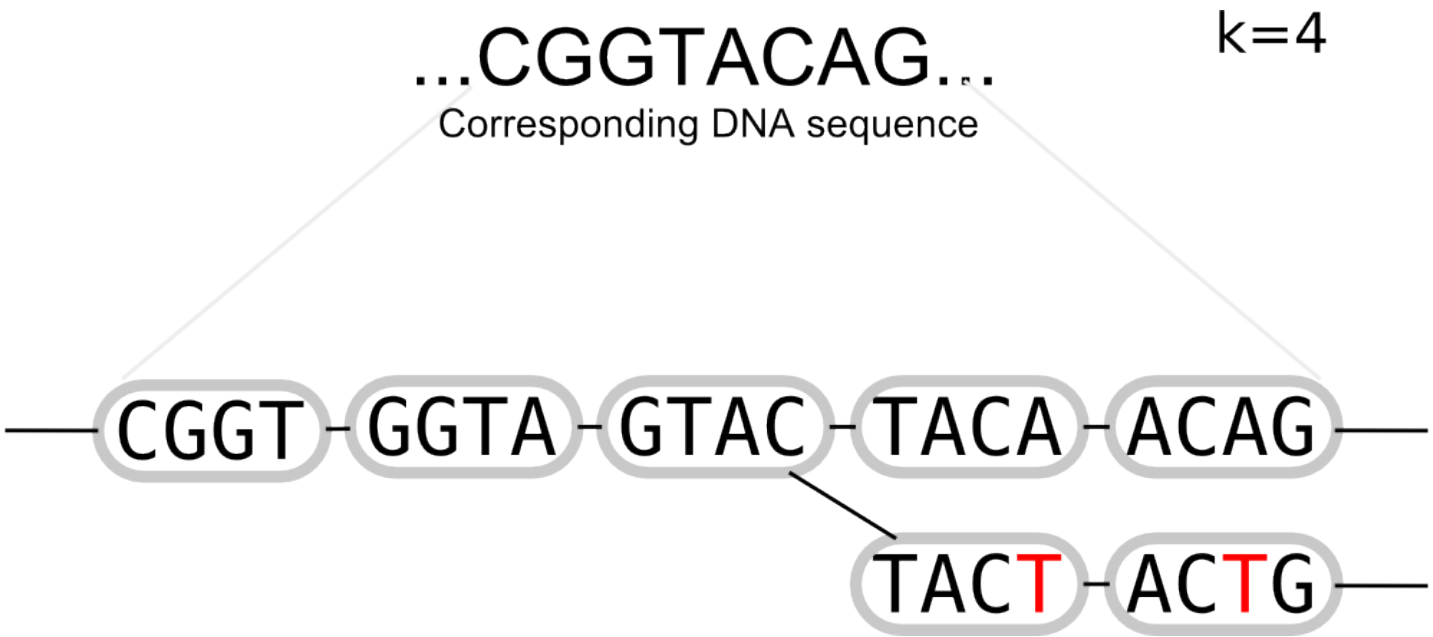
k-mers

A k-mer is a substring of length k of a read.
All the k-mers of a set of reads form its *set of k-mers*.

De Bruijn graphs

For a given k, the De Bruijn graph $\mathcal{G}$ of a set of reads $\mathcal{R}$ is a graph (V, E) such that E is the set of k-mers of $\mathcal{R}$ and such that $(u, v) \in V$ if and only if u and v overlap by $k - 1$ bases.

An example De Bruijn graph



SNPs: a genomics problem

The *genome* of an individual is made of *chromosomes*.
A chromosome $\rightarrow$ a DNA sequence
chromosomes are often *paired*.

Single Nucleotide Polymorphism (SNP)

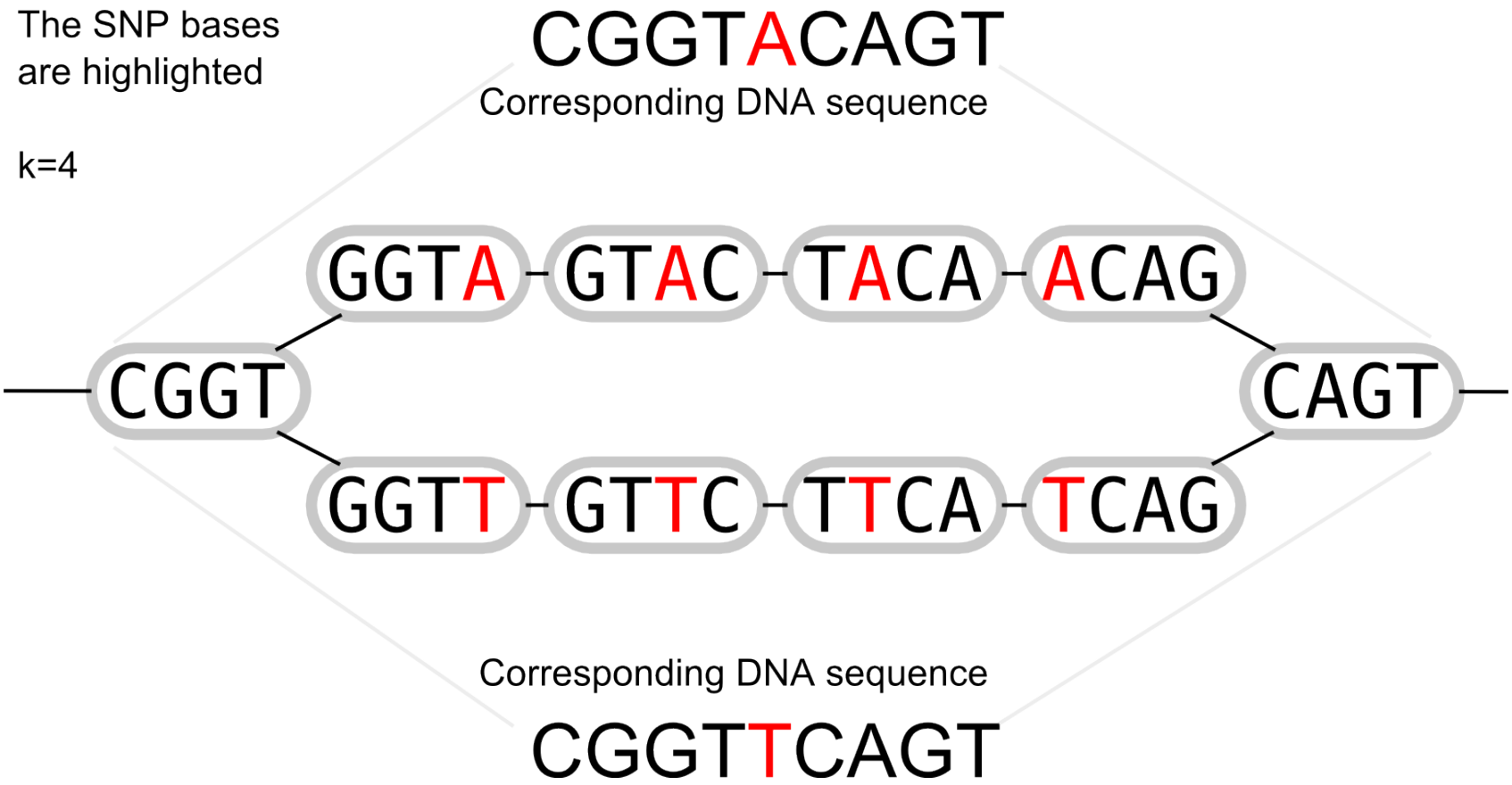
A Single Nucleotide Polymorphism or SNP is a variation of a single base (also called a *nucleotide*) between two paired chromosomes or between two individuals of the same species.

Goal of the internship
$\rightarrow$ design a SNP-finding algorithm based on De Bruijn graphs

SNPs in De Bruijn graphs

The SNP bases are highlighted

k=4



Hybrid parallel programming

Hybrid parallel programming

Mixing shared memory and message passing in a parallel algorithm.

- Message passing $\Longrightarrow$ *overhead*
- Shared memory $\Longrightarrow$ specific architecture
- Hybrid computing:
  - has low overhead
  - works with most cluster architectures
- Well-adapted to many bioinformatics clusters (several 48-cores machines, for instance)

Outline of the algorithm

To solve the SNP detection problem using De Bruijn graphs and hybrid parallel programming we have designed the following algorithm:

1. extract the k-mers from the set of reads and distribute them among the nodes
2. compute adjacency information for each k-mer
3. look for SNPs in the built De Bruijn graph

Each step will use hybrid parallelism:
$\rightarrow$ work will be divided among message-passing processes
$\rightarrow$ each process will then divide work among threads

Distribute k-mers among the nodes

The set of reads is divided among the processes.
Each process divides its reads among its threads.
Each thread executes the following algorithm:

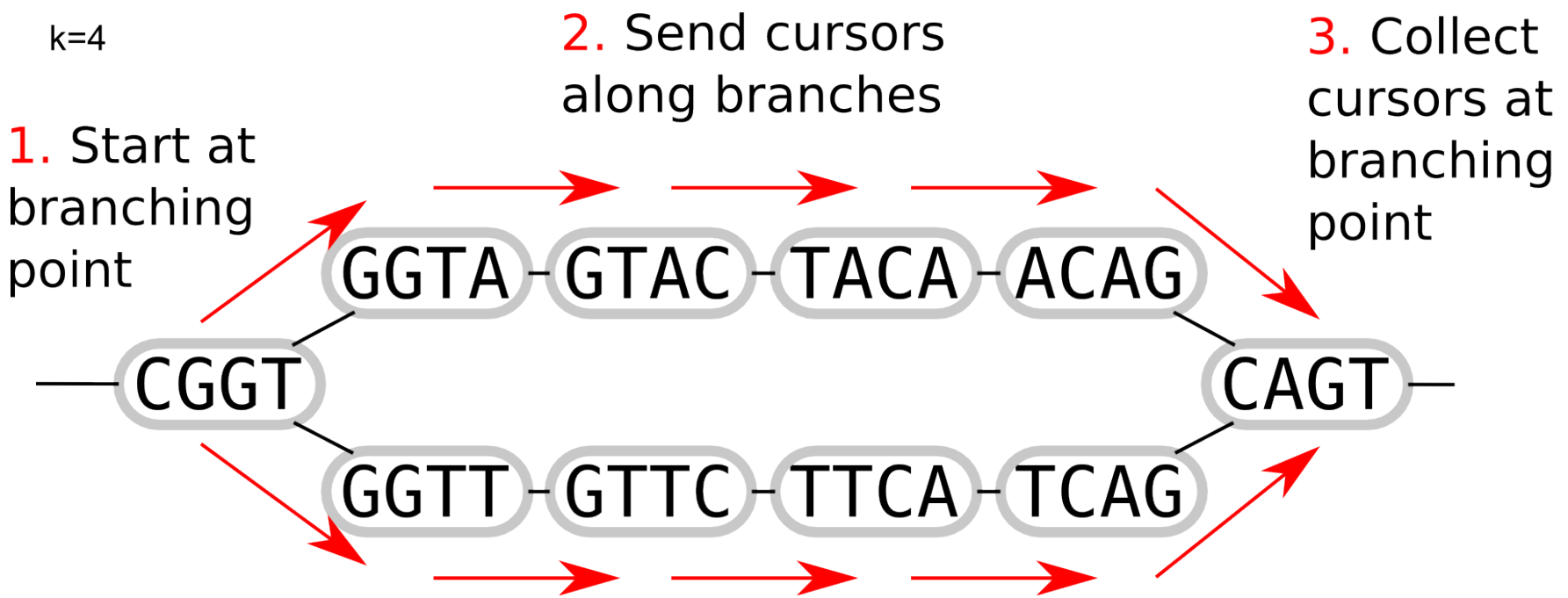
1. break each read into k-mers
2. send each k-mer to the process given by a hash function on k-mers
3. add each received k-mer to a hashtable in the shared memory of the process

Build the De Bruijn graph

The set of computed k-mers of each process is divided among its threads.
Each threads executes the following algorithm:

1. send each k-mer to the owners of its 8 possible neighbors; a property of the hash function ensures those neighbors will belong to a maximum of 2 different processes
2. for each received k-mer
   - if a neighbor u is present in the hashtable, update adjacency information for u
   - if a *branching point* is detected while updating adjacency information, add it to a branching point hashtable in shared memory

Find the SNPs



3'. Discard cursors that have done too many steps

Implementation using MPI and OpenMP

Implementation was done using:

- *C++*
- *MPI* for the message-passing part
- *OpenMP* for the shared memory part

The program was called HyBu.
First two steps of the algorithm: implemented and tested
Last step of the algorithm: work in progress

Benchmarks using the LBBE's cluster

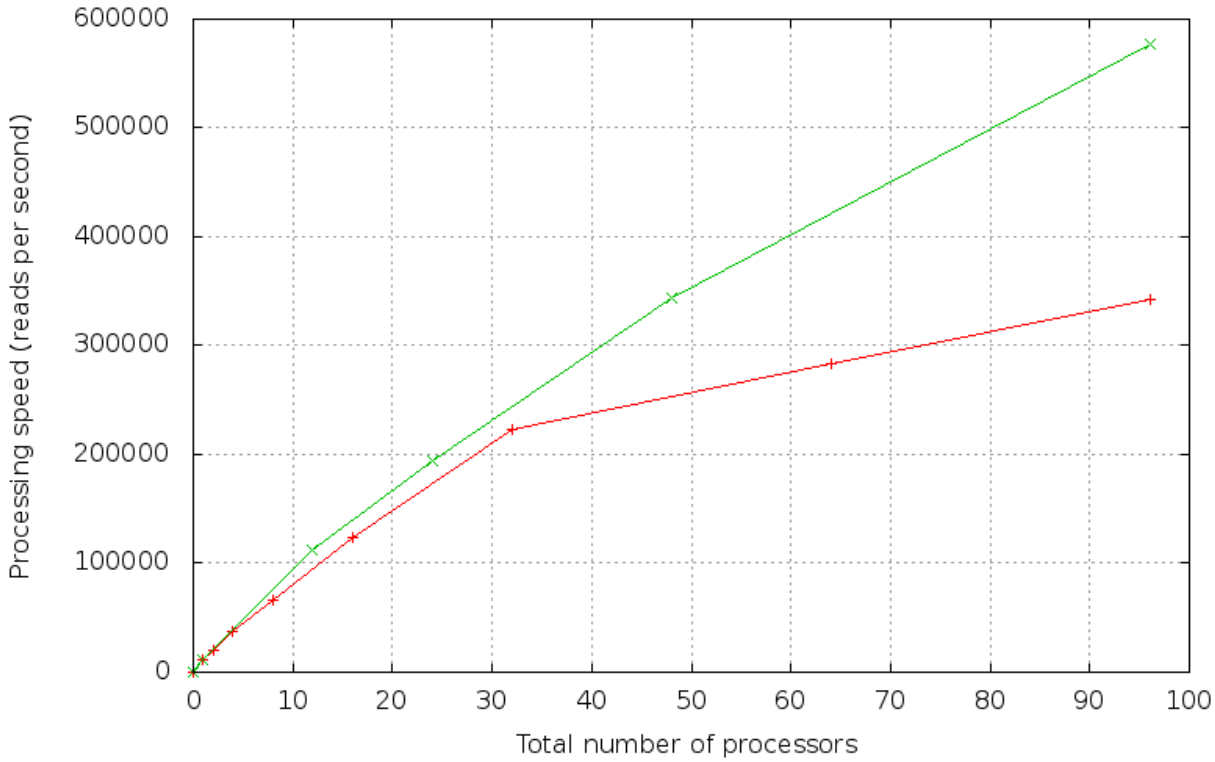


Figure: De Bruijn graph building on two 48-cores nodes.
Red curve: one process per node.
Green curve: 6 processes par node.

Conclusions

- successful design and implementation of an hybrid SNP detection algorithm
- tests on the LBBE's cluster show good scalability up to 96 processors
- gains from hybrid programming not obvious

Thank you for your attention.