Local sequence alignment for an associative model of parallel computation

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Introduction

The goal of sequence alignment is to find similarity between the different strings of genetic information.

similar characters → similar structure → similar function

Ancestral Relationships
Gene Functionality
Aid in Drug Discovery

Local Sequence Alignment

Optimization Problem

- Maximize sub-sequence similarity (**local alignment)**

Smith Waterman algorithm

- Exact algorithm[1], finds highest scoring local alignment
- Slow, uses dynamic programming method (DP) to get exact answer
- Heuristic algorithms such as BLAST are faster, but not always the best alignments

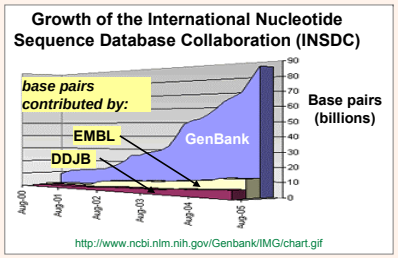


Fig. 1. Exponential growth of sequence data means more to align with; speed as well as quality of information is vital.

Parallel Alignment Goals

Produce More Information

- Return top *k*-ranked alignments
- The *k* alignments are non-overlapping / non-intersecting

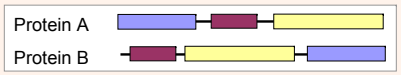


Fig. 2. Proteins with three local non-intersecting alignments.

Fast Local Alignments

- Find all *k* alignments in the same time it takes to find a single alignment

Parallel Model

The ASsociative (ASC) and Multiple ASsociative Computing (MASC) models[2] are SIMDs with an associative property and some additional hardware features.

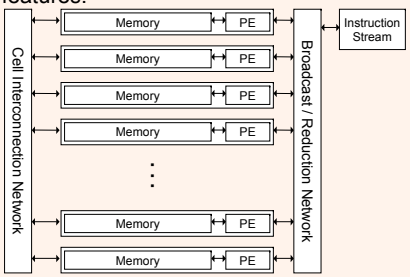


Fig. 3. A high-level view of the ASC model. The MASC model includes more than one instruction stream.

ASC / MASC features

- Fast processing
- Constant time search/respond ops
- Constant time global reduction ops: max/min of processing elements (PEs)
- A base of existing algorithms[3]
- Existing programming language and emulator

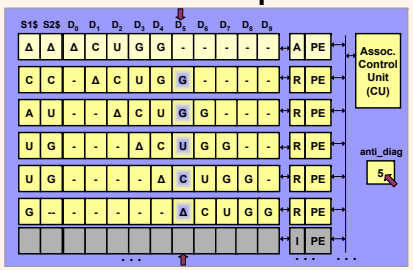
Associative Adaptation

Weights for the following examples:
Gap Insert: 3; Gap Extend: 0
$d(S1_i, S2_j) = 10$ when $S1_i = S2_j$
$d(S1_i, S2_j) = 10$ when $S1_i \neq S2_j$

PE i[$] index / S1	PE j[$] index / S2	0 Δ	1 C	2 U	3 G	4 G
0	Δ	0	0	0	0	0
1	C	0	10	7	7	7
2	A	0	7	7	4	4
3	U	0	7	17	14	14
4	U	0	7	17	14	14
5	G	0	7	14	27	24

Fig. 4. Traditional Smith-Waterman DP table. The dependency free anti-diagonal that the ASC algorithm executes in parallel is highlighted.

Associative Example



S1: CAUUG Alignment: CAUUG
S2: CUGG C- - -UGG

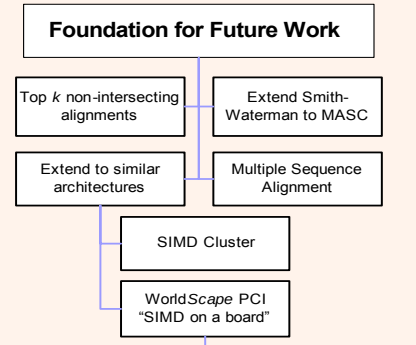
Fig. 5. Mapping the Smith-Waterman algorithm on ASC.

Active PEs hold one character of S1 and S2. D is a parallel array of size |S1| + |S2|. D's subscript represents a particular anti-diagonal.

S2 is stored in a systolic fashion to allow parallel computation of the values along the anti-diagonal.

Active PEs compare their S1 value with each particular D_j value to compute the function *d* listed above (not shown).

Foundation for Future Work



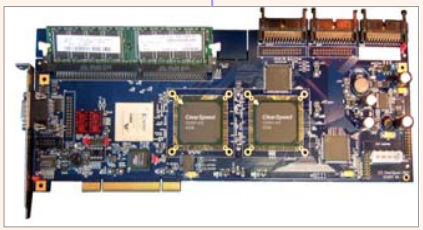


Fig. 6. World*Scape* Dual 64 PCI SIMD Board with 50 GFLOPS performance.

Intent

- Provide fast, accurate, more detailed alignments that aid in bioinformatics
- Work towards identifying regulatory regions in genes and response elements

References

[1] Goto, O. "An Improved Algorithm for Matching Biological Sequences." *J. of Molecular Biology* 162, 705-708, 1982.
[2] Potter, J., J. Baker, A. Bansal, S. Scott, C. Leangsuksun, and C. Asthagiri. "ASC: An Associative Computing Paradigm." *IEEE Computer*, 27(11): 19-25, November, 1994.
[3] Esenwein, M., J. Baker, "VLCD String Matching for Associative Computing and Multiple Broadcast Mesh", *Proc. of 9th IASTED International Conf. on Parallel and Distributed Computing Systems*, 69-74, 1997.

For further information

Please contact ssteinfa@cs.kent.edu. More information on this and related projects can be obtained at http://www.cs.kent.edu/~parallel.