Parallel large scale inference of protein domain families

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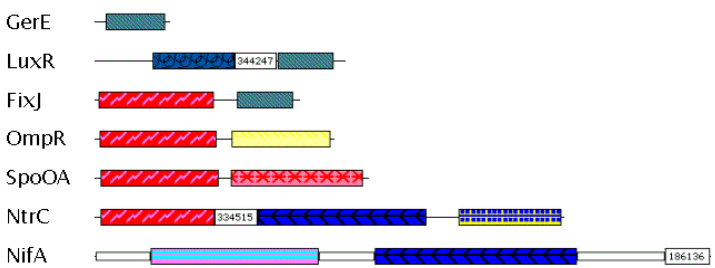
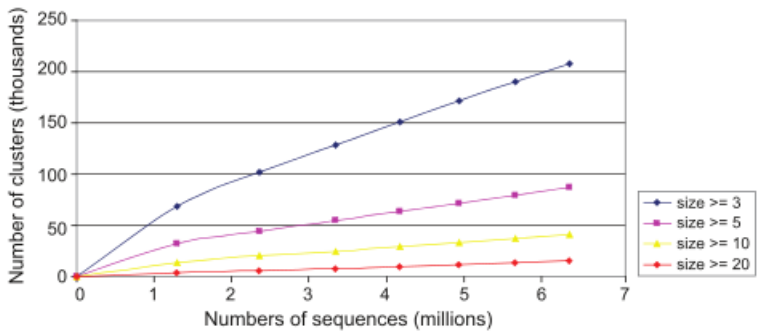
Protein modularity

- Domains: conserved units of protein structure
- Proteins often composed of combinatorial arangement of domains





Yooseph *et al.* 2007

MPI_Mkdom2

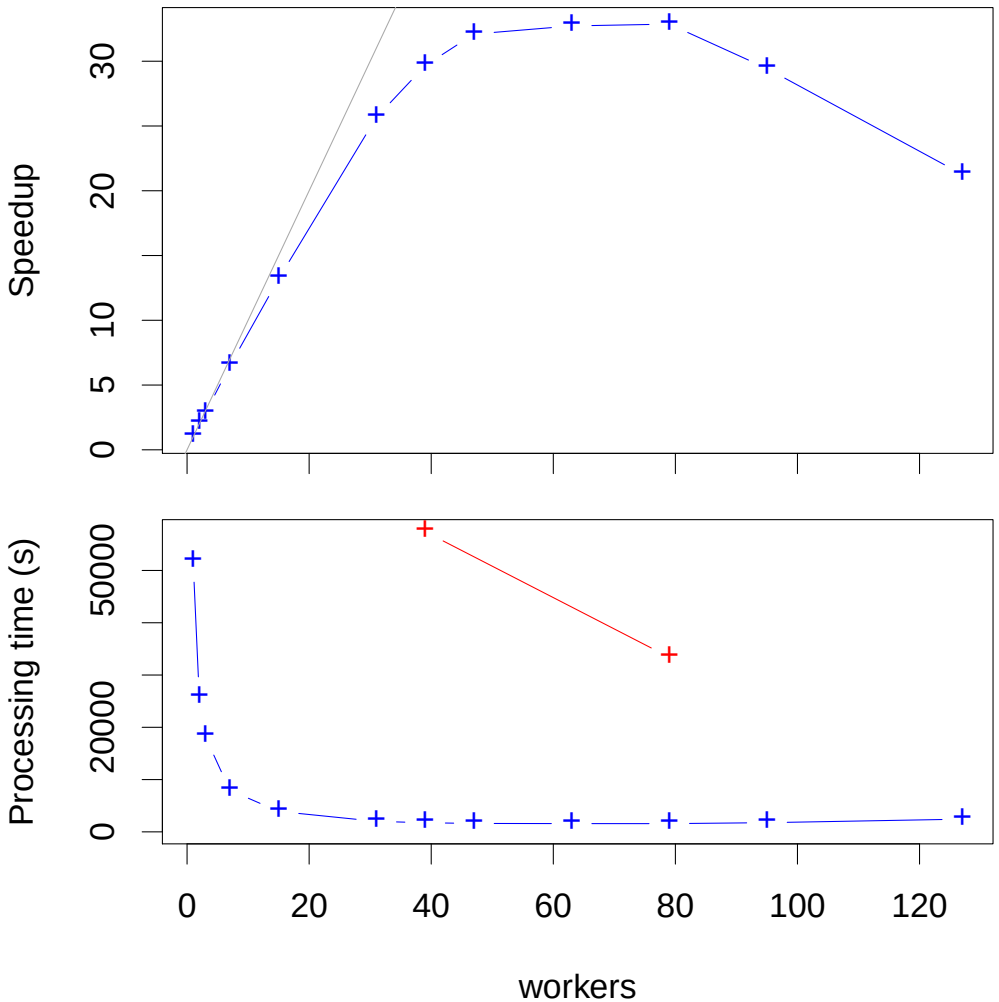
Mkdom2

- Greedy algorithm
- At each step: create a family around the shortest sequence.

MPI_Mkdom2

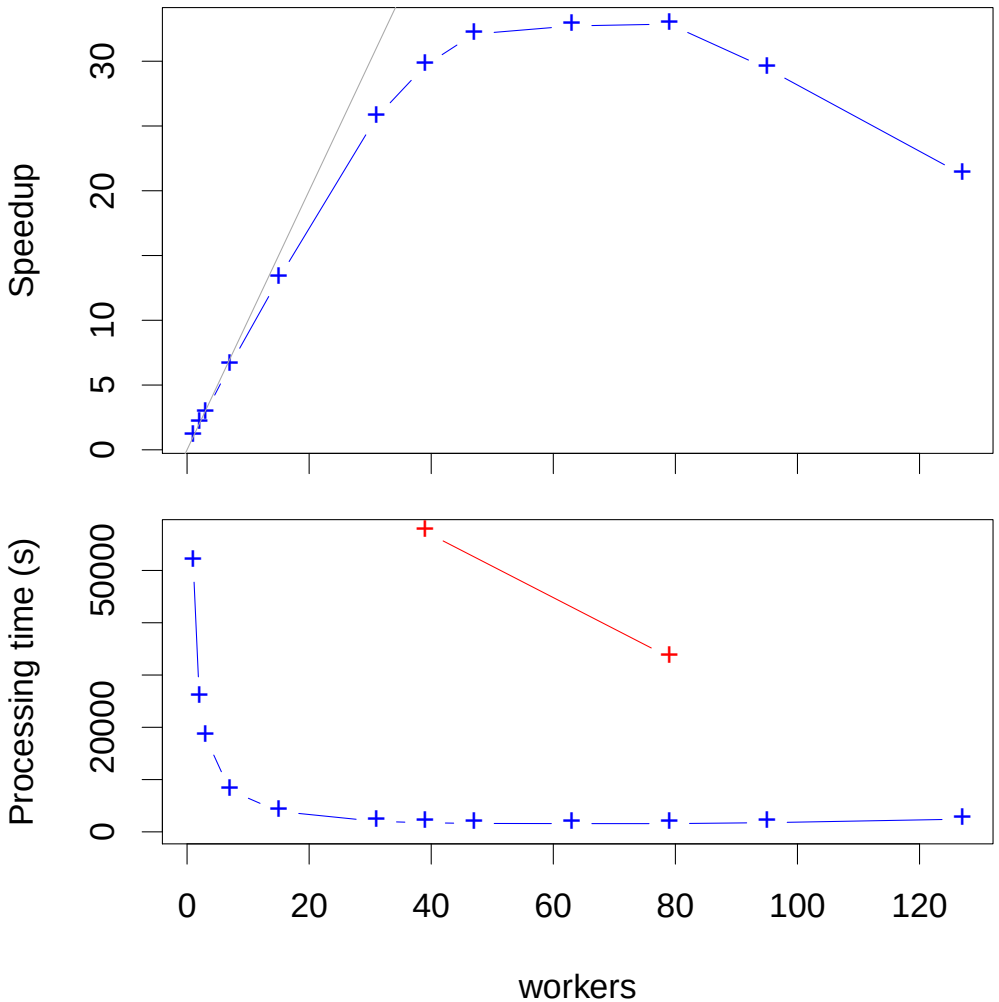
- Targeted at clusters, grids.
- Process multiple queries at once, check for overlapping results afterwards
- Try to avoid running interdependent queries on the basis of a global comparison.
- Handle large variations in query processing times.

Speedup



69,621 sequence dataset

Speedup



69,621 sequence dataset

556,964 sequence dataset

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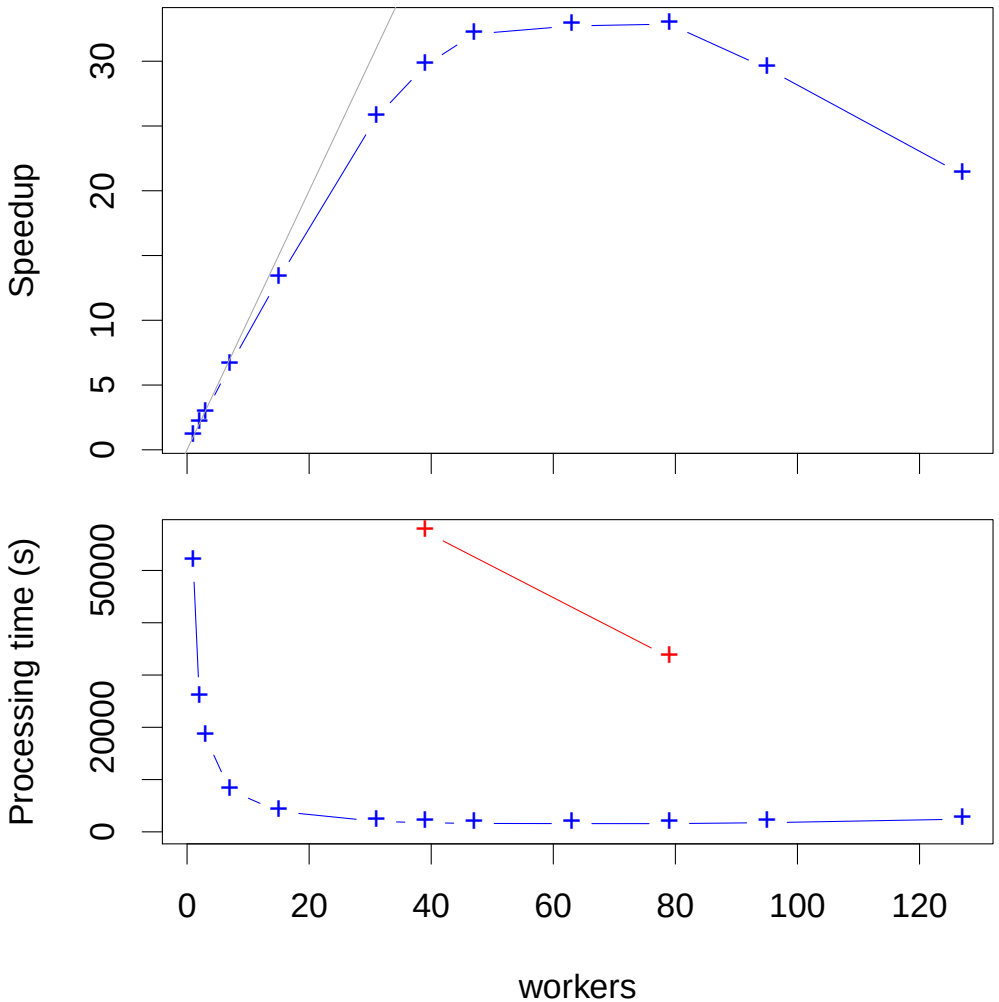

69,621 sequence dataset

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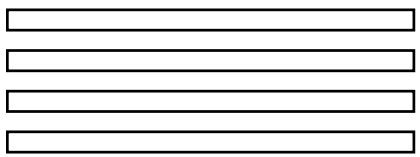
The larger the database, the larger the speedup

Comparing clusterings

- Need to compare both domain extents and domain clustering.



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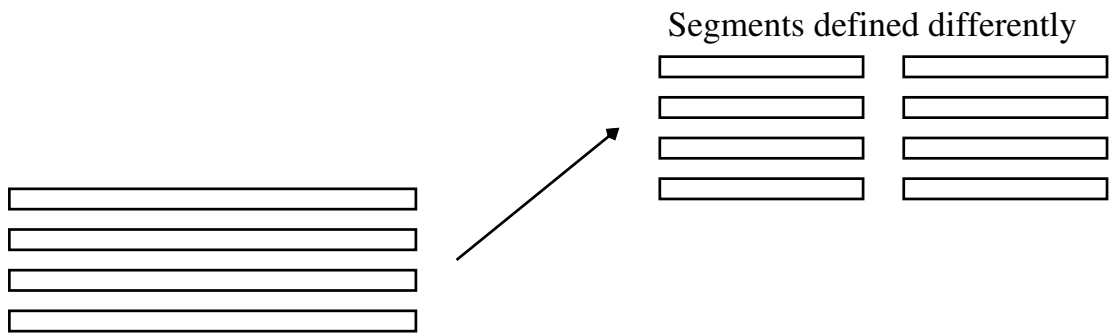

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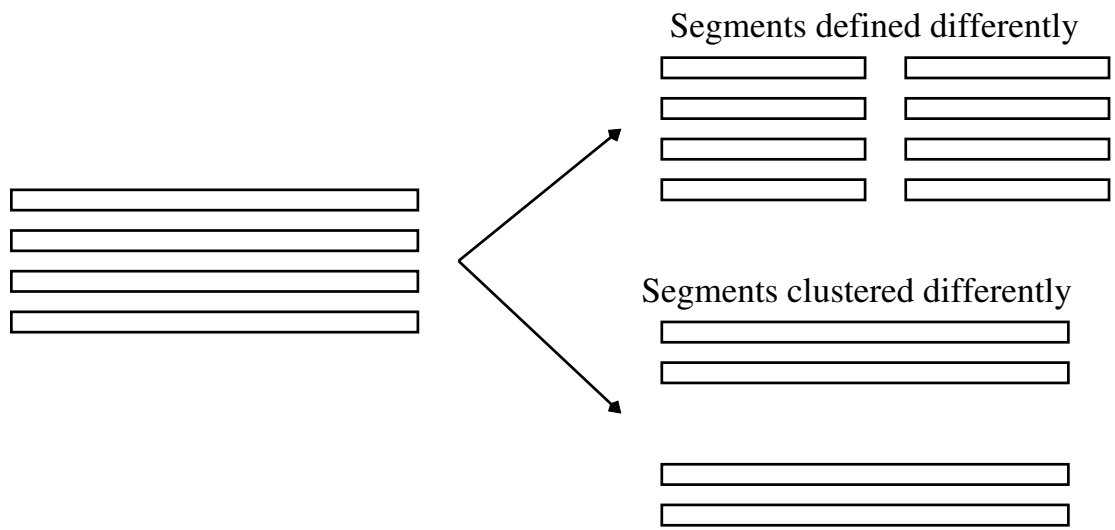
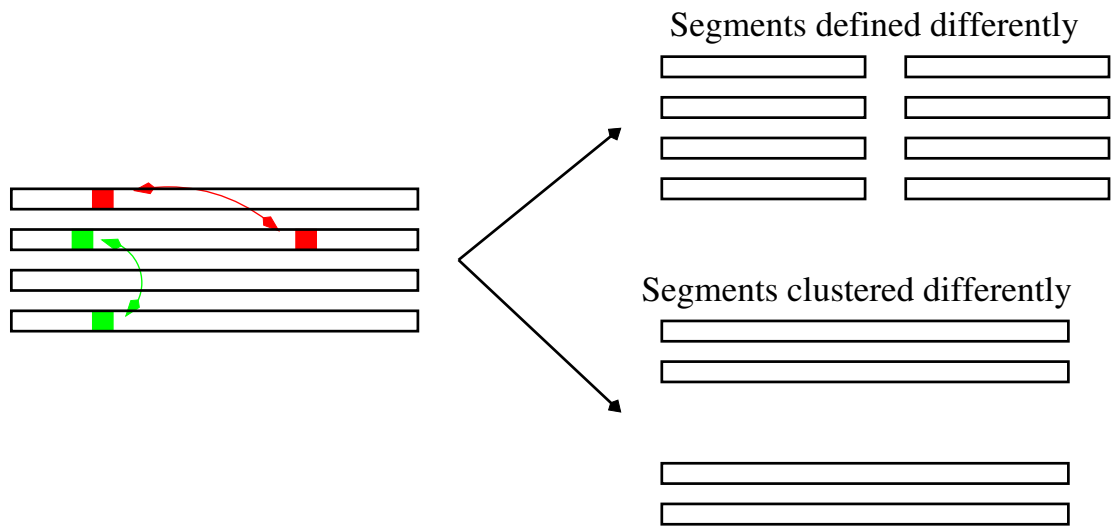


Comparing clusterings

- Need to compare both domain extents and domain clustering.
- Wallace index: counting preserved pairs.



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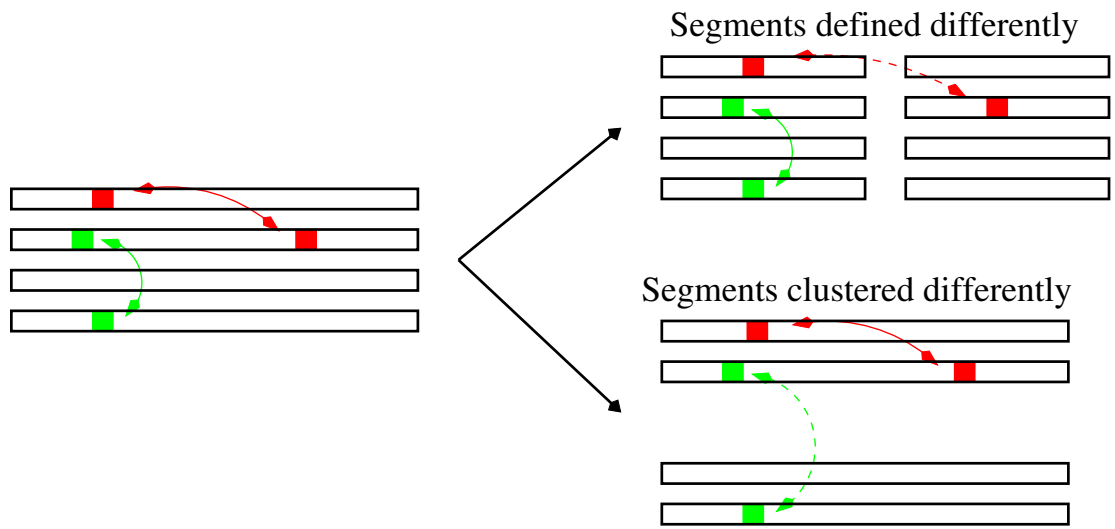
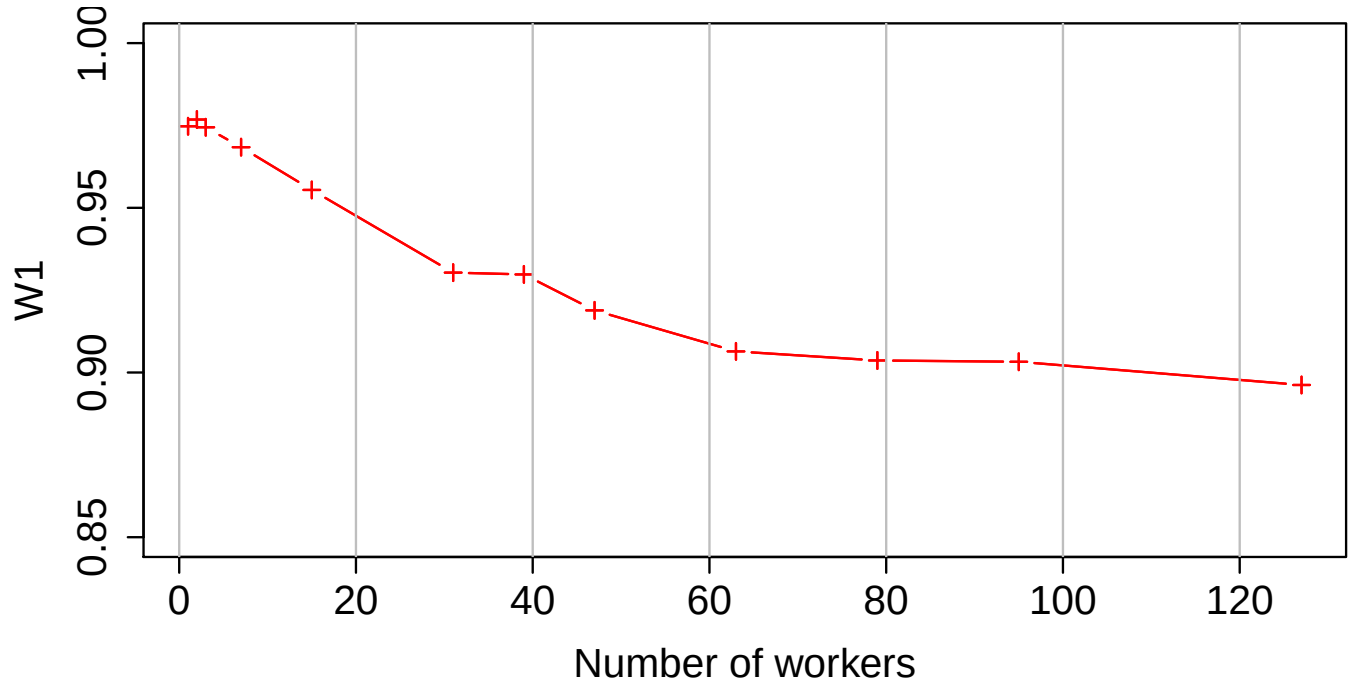


Result validation: comparing parallel and sequential results



- Clustering reasonably preserved, even with a large number of workers.
- Compute ProDom 2010 (set of 6,118,869 sequences, in progress)