## A well-separated pairs decomposition algorithm for kd-trees implemented on multi-core architectures

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GridPP
UK Computing for Particle Physics

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## Motivation

- A problem
- Given a set $P$ of $n$ points in $R^{d}$ :
- find the two closest points to each other belonging to $P$ (e.g. Eppstein);
- for each $q \in P$, find its closest neighbour in $P-q[6]$;
- find all $k$ nearest neighbours of each $q \in P$ [4].


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- find all $k$ nearest neighbours of each $q \in P$ [4].
- Theoretical limits
- all solvable in $O(n \log n)$ work if an $O(n \log n)$ work algorithm spatial indexing is available.
- parallel algorithms using $p$ processors and $O(n \log n)$ work theoretically available (Callahan in [4]).


## Good for HEP and Physics?

- Multivariate analysis for TMVA in ROOT uses $k$ nearest neighbours search. Repeated analysis might benefit of k -d-tree algorithm with $O(n \log n)$ work with decent scalability.
- Track reconstruction by joining compatible triplets has been approached in CMS using $k$-d-trees and cellular automata. Even the the simulation of celular automata might demand multidimensional data organisation when the number of dimensions increase.
- N-body computations based on Barnes-Hutt or Fast Multipole Method in general depend on tree methods.
- N-point correlation functions have been tackled in Astronomy by the use of search in $k$-d-trees [5].


## Proposed solution

- K-d-tree based solution built on
- fair split that will lead to Well Separated Pair Decomposition;
- balanced partitioning giving $O(\log n)$ height independent of input;
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- Implementations in the paper
- First implementation of a parallel WSPDP algorithm.
- Possibly first implementation of a parallel $k$ - $d$-tree (Lisp, C/OMP, C++/TBB.)
- Parallel scalable implementation of Kth-selection algorithm


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## Quadtrees: a choice for parallel spatial indexing?



- each node partitions a set of points by all $d$ attributes, each representing one dimension. partitions for the set in question
- Samet [8]: used by all published works on parallel spatial indexing.
- disadvantages:
- curse of dimensions: number of empty (or nearly empty) partitions increasing fast with dimensions.
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## K-d-trees: questions

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- Each nodes defines a discriminator (splitting dimension)
- Each discriminator has an associated cut value: the dimension value of the points in the subset being partitioned
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- Each discriminator has an associated cut value: the dimension value of the points in the subset being partitioned
- discriminators cycle through the $k$ dimension on the path from root to leaf nodes
- Disadvantages
- cycling through dimensions can still lead to leaf depth unbalancing
- choice of cut value, a problem to be solved
- distribution of work on $p>1$ processors scenario can be complicated due to recursive nature
- work balancing still a problem


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(3) Parallel k-d-trees

4 What could go wrong?

- Splitting criteria
- each node defines a range of the space
- split close to the middle of the range
- split should guarantee either:
- balanced distribution of points for children nodes
- or total of comparisons on the order of the size of the node being split
- Fair split target balanced number of comparisons in sequential split
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- split adapts Bentley's "burning the candle from both ends" algorithm [1].
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- Problem for parallel algorithm
- split must "guess" (or brute force search) slabs of splitting
- Callahan does "hand waving argument" to show that it is possible
- Har-Peled [6] proposes splitting based on one of
- radix splitting
- k-enclosing disk splitting


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- asynchronously parallel algorithm: full use of all processors as they become available.


## Splitting for balanced k-d-tree

- Split close to the median.
- Based on Blum, Floyd, Pratt, Tarjan algorithm of kth-selection
- Parallel map blocks of 5 elements to its median
- Recursion until block of up to 5 central elements is found.
- Easy elimination of recursion.
- Guaranteed time in $O(n)$.
- Median of final blocks always greater than $\frac{3 n}{10}$ and less than $\frac{7 n}{10}$ elements of initial set.
- Additional element from final block used for a two pivots split.
- Option for split at the middle of the range based on A. Moore [7].


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- split in three steps
- parallel search for dimension to split
- parallel search for splitters using median of 5
- parallel split adapting Bentley's invariant for one pivot to a two pivot split.
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- Short queue split:
- Each process available takes one node to split with same algorithm as long queue.
- Based on gcc (-fopenmp) 4.6, Ubuntu 13.04, Intel xeon 5660.
- Sets with up to $2^{16}$ points processed asynchronously with one processor.
- Speed-up and efficiency shown in the table only for the 1572864 set.

| points in 3-d | 1 proc | 4 procs | 8 procs | 12 procs |
| ---: | ---: | ---: | ---: | ---: |
| 65536 | $0.856 s$ | $0.868 s$ | $0.857 s$ | $0.854 s$ |
| 252144 | $3.206 s$ | $1.337 s$ | $1.235 s$ | $1.391 s$ |
| 524288 | $6.551 s$ | $2.545 s$ | $1.338 s$ | $1.512 s$ |
| 786432 | $9.724 s$ | $3.991 s$ | $2.781 s$ | $1.862 s$ |
| 1572864 | $18.43 s$ | $7.515 s$ | $4.532 s$ | $3.623 s$ |
| $S_{p}$ | 1 | 2.45 | 4.14 | 5.08 |
| $E_{p}$ | 1 | 0.61 | 0.51 | 0.42 |

- Speed-up $S_{12}=\frac{T_{12}}{T_{1}}$
- Efficiency $E_{12}=\frac{S_{12}}{12}$


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- Careful! Categorization pattern can be very costly!
- Is WSPDP too heavy?
- Yes, when number of dimensions increase [6].
- Sequential approximation algorithm available. Parallel?


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- Parallel processing in the long queue not decoupled enough for distributed memory will demand (maybe too many) data movements.
- Extensive testing/tuning for algorithm with an initial phase of sampling to distribute points when running on cluster.
- MIC computation could be more feasible due to lower communication costs.


## Conclusion

- The simple structure of $k$-d-trees offers promissing alternatives regarding:
- Restricting the height of resulting trees.
- balancing of work load in parallel implementation.
- Challenges that need to be worked:
- Irregular parallelism of present algorithm not the best regular SIMD as found in GPUs.
- Improving memory management in parallel execution might result in huge gains in computing time and efficiency.
- Scheduling of synchronised steps affects time and efficiency.


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