'votess: A multi-target, GPU-capable, parallel Voronoi tessellator'

Samridh Dev Singh [1], **Chris Byrohl** [2], **and Dylan Nelson** [2]

1 Grinnell College, 1115 8th Avenue, 50112 Grinnell, United States of America **2** Heidelberg University, Institute for Theoretical Astronomy, Albert-Ueberle-Str. 2, 69120 Heidelberg, Germany

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Statement of need

A Voronoi tessellation is a spatial decomposition that partitions space into a set of convex hulls based on proximity to a seed points with interesting to the applications in biology, data science, geography, and physics. One compute intensive application is its use in astrophysics, such as the analysis of matter distribution (Weygaert, 1994), optimal transport theory for early-universe reconstruction (Levy et al., 2021), and in observational data analysis and numerical simulations of cosmic structure formation (Springel, 2010).

The increasing size of datasets produced today have underscored the need for more efficient algorithms to both generate and analyse these datasets, and the rise of heterogenous computing facilities would enable such new algorithms to be run. There do exist several sequential and parallel implementations of the Voronoi diagram problem (Marot et al., 2019) (Wu et al., 2023) (The CGAL Project, 2018) (Inria, 2018), however, they are mostly restricted to CPU or specific GPU architectures, thus limiting their potential as a portable multi-architecture algorithm.

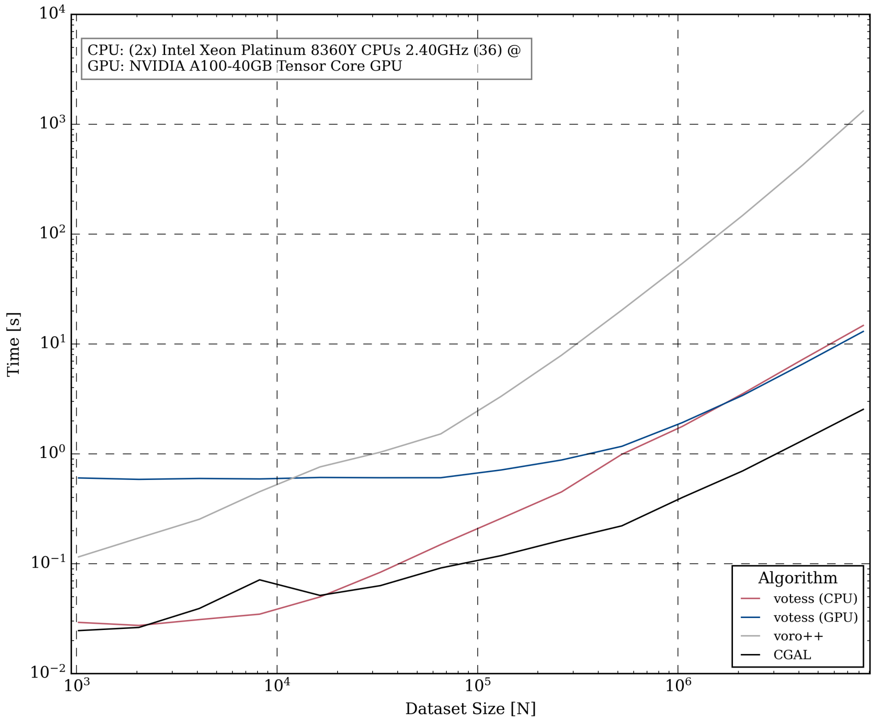
Summary

`votess` is a library, implementing Ray's meshless algorithm (Ray et al., 2018), for computing parallel three dimensional Voronoi tessellations using the C++/SYCL framework for CPU, GPUs and other future architectures.

One advantage of this algorithm is the ability for each cell to be computed independently (Ray et al., 2018), making it suitable for parallel execution. It also produces the geometry of the Voronoi cells via their neighbor connectivity information, rather than a full combinatorial mesh data structure, thus making it more ammenable to data parallel architectures than alternatives such as sequential insertion or the Bowyer-Watson algorithm (Bowyer, 1981) (Watson, 1981).

The core method of `votess` consists of two main steps. First, the input set of points is sorted into a grid, and a k-nearest neighbors search is performed. Once the k nearest neighbors are identified for each point, the Voronoi cell is computed by iteratively clipping a bounding box using the perpendicular bisectors between the point and the identified neighbors. A *security radius* condition (Lévy & Bonneel, 2013) ensures that the resulting Voronoi cell is valid, and if the cell cannot be validated, an CPU fallback mechanism is used.

Performance



In Figure 1, we show its performance compared to two other single-threaded Voronoi tessellation libraries: `CGAL` and `Voro++`. Both are well-tested and widely used. CGAL implements Voronoi Tesellations through a Delaunay mesh using the CPU in parallel (The CGAL Project, 2018), while `Voro++` computes three-dimensional Voronoi tessellations in a single core via a cell-based computation approach that is well-suited for physical applications (Rycroft, 2009). The benchmark uses a `float32` uniformly distributed dataset, as it is currently the simplest to test. From the results of (Ray et al., 2018), this dataset would provide the lowest performance, but higher than clustered datasets: datasets currently beyond the scope of the current version.

Other Multithreaded Voronoi tesellelation codes exist, including `ParVoro++` (Wu et al., 2023), and `GEOGRAM` (Inria, 2018). However, they do not natively support GPU architectures, and we are unable to benchmark them.

From the graph above, `votess` outperforms the single-threaded alternative, however, when compared to the established CGAL, both the CPU and GPU version falls short by around a factor of 6. Currently the problem is being addressed, and future optimizations should close the gap.

Features

`votess` is designed to be versatile. It supports various outputs, including the natural neighbor information for each Voronoi cell. This is a 2D jagged array of neighbor indices of the sorted input dataset.

Users can invoke `votess` in three ways: through the C++ library, a command-line interface `clvotess`, and a Python wrapper interface `pyvotess`. The C++ library offers a simple interface with a `tessellate` function that computes the mesh. The Python wrapper, mirrors the functionality of the C++ version, with native numpy array support, providing ease of use for Python-based workflows.

The behavior of `votess` can be fine-tuned with run time parameters in order to (optionally) optimize runtime performance.

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