The Journal of Open Source Software

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

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DOI: 10.xxxxxx/draft

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Submitted: 01 January 1970
Published: unpublished

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Statement of need

The Voronoi tessellation is a spatial decomposition that partitions space into a set of convex hulls based on proximity to a discrete set of seed points. It is an interesting problem due to the applications in biology, data science, geography, and physics. A few examples exist in computational cosmology, initally pioneered by van de Weygeart [@], in the form of Optimal transport theory (elucidate?) [@], or in observational data analysis as well as 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 exists 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 for computing parallel 3D Voronoi tessellations on heterogeneous platforms, from CPUs to GPUs to future accelerator architectures. To do so, it uses the SYCL single-source framework abstraction in the C++ language. `votess` was designed to be portable yet performant, accessible to both developers and users with several easy-to-use interfaces.

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.

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). Additionally, a grid based datastructure for the all-k-nearest-neighbors sub problem, succeeded with the iterative clipping enables better caching behaviour on the GPU.

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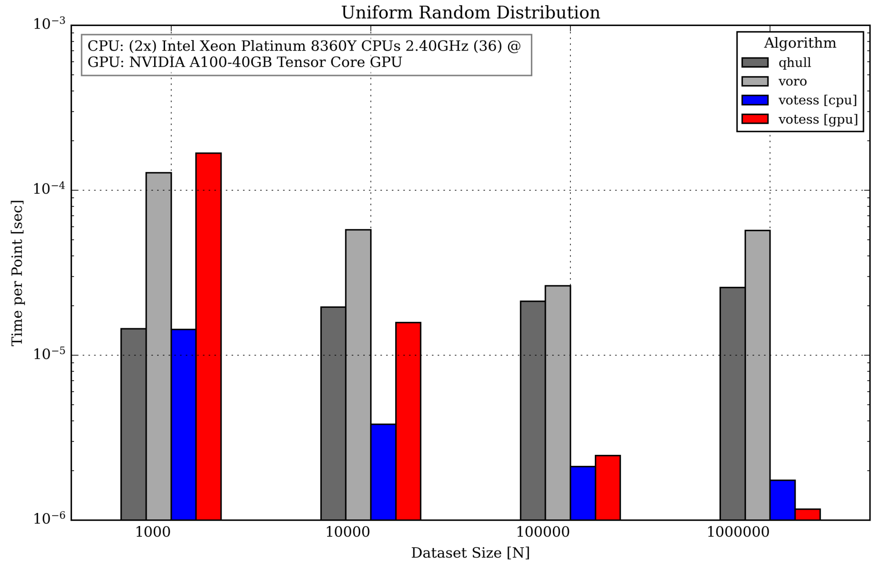
Performance



From the graph above, `votess` outperforms single-threaded alternatives.

In Figure 1, we show its performance compared to two other single-threaded Voronoi tessellation libraries: `Qhull` and `Voro++`. Both are well-tested and widely used. `Qhull` is a computational geometry library that constructs convex hulls and Voronoi diagrams using an indirect projection method (Barber et al., 1996), while `Voro++` is a C++ library specifically designed for three-dimensional Voronoi tessellations, utilizing a cell-based computation approach that is well-suited for physical applications (Rycroft, 2009).

We find that `votess` performs best on GPUs with large datasets. The CPU implementation can outperform other implementations by a factor of 10 to 100.

Multithreaded Voronoi tessellelation codes do exist, and these include `ParVoro++` (Wu et al., 2023), `CGAL` (The CGAL Project, 2018), and `GEOGRAM` (Inria, 2018). However, they do not natively support GPU architectures.

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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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Acknowledgements

CB and DN acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG) through an Emmy Noether Research Group (grant number NE 2441/1-1).

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