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

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Statement of need

The Voronoi tessellation is a spatial decomposition that uniquely partitions space into convex sub-regions based on proximity to a discrete set of generating points. It is widely used across scientific domains. In astrophysics, Voronoi meshes are used in observational data analysis as well as numerical simulations of cosmic structure formation (Springel, 2010). The increasing size of modern datasets has underscored the need for faster, more efficient algorithms and numerical methods. The rise of powerful many-core CPU and GPU architectures has greatly increased the available computational power.

However, most existing implementations of Voronoi tessellations are tailored to specific architectures, limiting their portability. Additionally, classic sequential insertion algorithms have difficulty using multi-core systems in a fully parallel manner. No general purpose, publicly available code capable of GPU-accelerated parallel Voronoi mesh generation in 3D space is available.

Summary

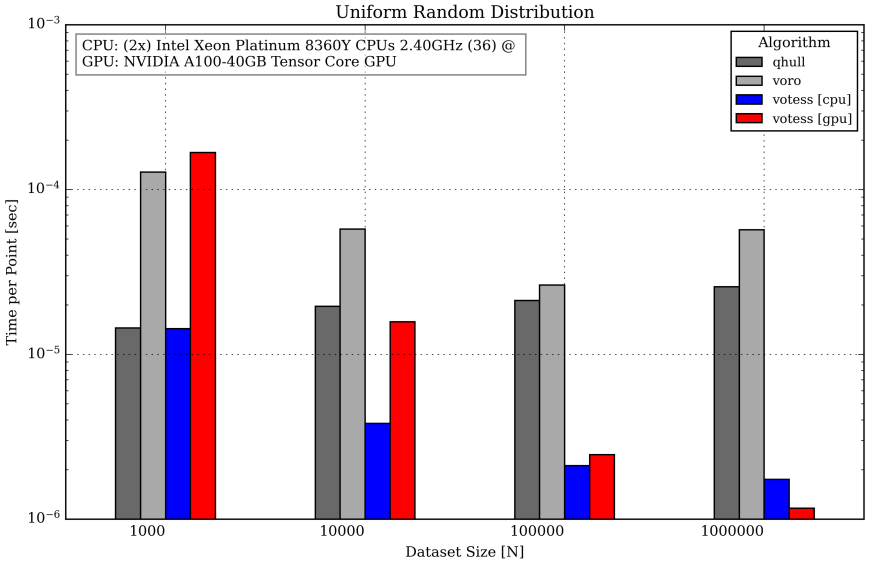
votess is a library for computing parallel 3D Voronoi tessellations on heterogeneous platforms, from CPUs to GPUs to future accelerator architectures. To do so, it uses the SYCL single-source framework abstraction. votess was designed to be portable yet performant, accessible to both developers and users with several easy-to-use interfaces.

The underlying algorithm computes the Voronoi mesh cell-by-cell (**?**). It produces the geometry of the Voronoi cells and their neighbor connectivity information, rather than a full combinatorial mesh data structure. This simplifies the method and makes it more ammenable to data parallel architectures than alternatives such as sequential insertion or the Bowyer-Watson algorithm.

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 its nearby neighbors. A "security radius" condition ensures that the resulting Voronoi cell is valid. If a cell cannot be validated, an automatic CPU fallback mechanism ensures robustness.

This efficient algorithm allows for independent thread execution, making it highly suitable for multi-core CPUs as well as GPU parallelism. This independence of cell computations achieves significant speedups in parallel environments.

Performance



As expected, `votess` can significantly outperform single-threaded lternatives.

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 large datasets. The CPU implementation can outperform other implementations by a factor of 10 to 100.

Multithreaded Voronoi tesellelation 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.

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, pyvotess, 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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