

'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

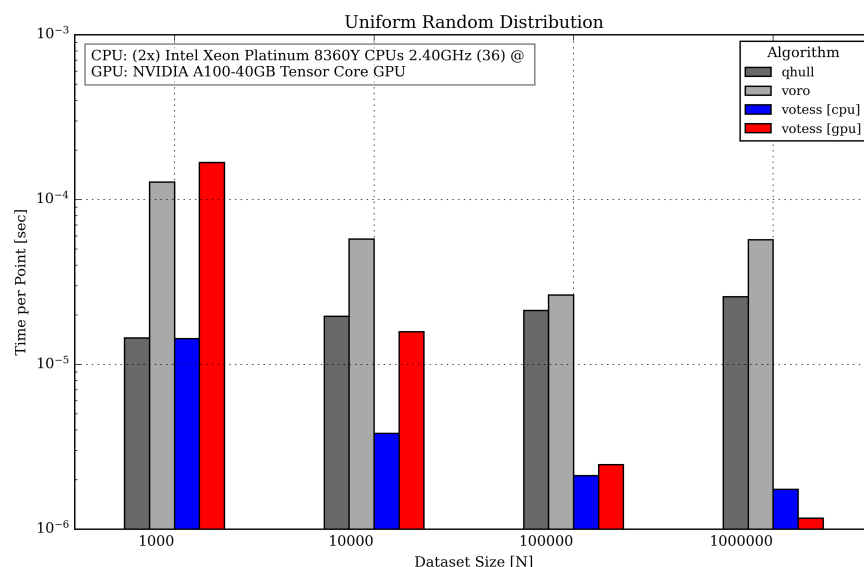
votess is a library for computing parallel 3D Voronoi tessellations on heterogeneous platforms, from CPUs to GPUs to future accelerator architectures. To do so, it uses the SYCL single-source framework abstraction. votess was designed to be portable yet performant, accessible to both developers and users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

The underlying algorithm computes the Voronoi mesh cell-by-cell ([Ray et al., 2018](#)). 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 amenable 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.

38 Performance



39

40 As expected, votess significantly outperforms single-threaded alternatives.

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

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

49 Multithreaded Voronoi tessellation codes do exist, and these include ParVoro++ (Wu et al.,
50 2023), CGAL (The CGAL Project, 2018), and GEOGRAM (Inria, 2018). However, they do not
51 natively support GPU architectures.

52 Features

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

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

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

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