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

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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.

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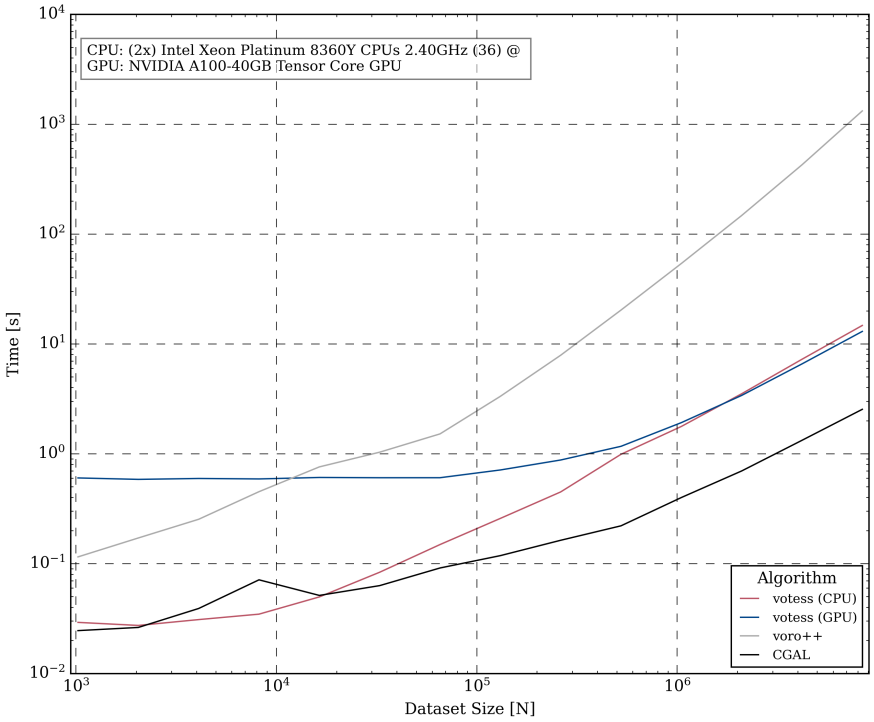
Performance



In Figure 1, we benchmark votess against two well-established libraries: CGAL, which builds parallel CPU-based Delaunay meshes (The CGAL Project, 2018), and Voro++, which performs single-core, cell-based 3D tessellations (Rycroft, 2009). All tests use a float32 white-noise dataset, which provide a worst case scenario for uniform datasets (Ray et al., 2018). The use of clustured datasets lies outside of both `votess` and the reference implementation (Ray et al., 2018), but remains in mind for future iterations of `votess`. Other Multithreaded Voronoi tesellelation codes exist, including `ParVoro++` (Wu et al., 2023), and `GEOGRAM` (Inria, 2018). However, they do not natively support GPU architectures, but are acknowledged as established alternatives.

From the graph above, `votess` outperforms `Voro++`, however, when compared `CGAL`, both the CPU and GPU version falls short by around a factor of 6. Ongoing optimizations for both backends are underway to close this 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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References

Bowyer, A. (1981). Computing dirichlet tessellations*. *The Computer Journal*, *24*(2), 162–166. https://doi.org/10.1093/comjnl/24.2.162

Inria, P. A.-G. (2018). *Geogram: A programming library of geometric algorithms*. http://alice.loria.fr/software/geogram/doc/html/index.html

Levy, B., Mohayaee, R., & Hausegger, S. von. (2021). A fast semidiscrete optimal transport algorithm for a unique reconstruction of the early universe. *Monthly Notices of the Royal Astronomical Society*, *506*(1), 1165–1185. https://doi.org/10.1093/mnras/stab1676

Lévy, B., & Bonneel, N. (2013). Variational anisotropic surface meshing with voronoi parallel linear enumeration. In X. Jiao & J.-C. Weill (Eds.), *Proceedings of the 21st international meshing roundtable* (pp. 349–366). Springer Berlin Heidelberg. ISBN: 978-3-642-33573-0

Marot, C., Pellerin, J., & Remacle, J.-F. (2019). One machine, one minute, three billion tetrahedra. *International Journal for Numerical Methods in Engineering*, *117*(9), 967–990. https://doi.org/https://doi.org/10.1002/nme.5987

Ray, N., Sokolov, D., Lefebvre, S., & Lévy, B. (2018). Meshless voronoi on the GPU. *ACM Transactions on Graphics*, *37*(6), 1–12. https://doi.org/10.1145/3272127.3275092

Rycroft, C. (2009). *VORO++: A three-dimensional voronoi cell library in c++*. https://doi.org/10.2172/946741

Springel, V. (2010). Moving-mesh hydrodynamics with the AREPO code. *Proceedings of the International Astronomical Union*, *6*(S270), 203–206. https://doi.org/10.1017/S1743921311000378

The CGAL Project. (2018). *CGAL user and reference manual* (4.12.1 ed.). CGAL Editorial Board. https://doc.cgal.org/4.12.1/Manual/packages.html#PkgSpatialSortingSummary

Watson, D. F. (1981). Computing the n-dimensional delaunay tessellation with application to voronoi polytopes*. *The Computer Journal*, *24*(2), 167–172. https://doi.org/10.1093/comjnl/24.2.167

Weygaert, R. van de. (1994). Fragmenting the universe. 3: The constructions and statistics of 3-d voronoi tessellations. *Astronomy and Astrophysics*, *283*(2), 361–406.

Wu, G., Tian, H., Lu, G., & Wang, W. (2023). ParVoro++: A scalable parallel algorithm for constructing 3D voronoi tessellations based on kd-tree decomposition. *Parallel Computing*, *115*, 102995. https://doi.org/10.1016/j.parco.2023.102995