PARAVT: Parallel Voronoi Tessellation code

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Abstract

We present a new open source code for massive parallel computation of Voronoi tessellations (VT hereafter) in large data sets. The code is focused for astrophysical purposes where VT densities and neighbors are widely used. There are several serial Voronoi tessellation codes, however no open source and parallel implementations are available to handle the large number of particles/galaxies in current N-body simulations and sky surveys.

Parallelization is implemented under MPI and VT using Qhull library. Domain decomposition take into account consistent boundary computation between tasks, and support periodic conditions.

In addition, the code compute neighbors lists, Voronoi density and Voronoi cell volumes for each particle, and can compute density on a regular grid.

Code implementation and user guide are publicly available at https://github.com/regonzar/paravt.

Keywords: methods: N-body simulations, large-scale structure of universe, Software and its engineering: Massively parallel systems

1. Introduction

The Voronoi Tessellation (\textsuperscript{Voronoi} \textsuperscript{1908}) technique define a cellular-like structure, where each particle is associated to a region (or Voronoi cell) in which any point inside this region is nearest to that particle than to any other.

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In the field of Astrophysics, in particular for N-body simulations, this is a very useful tool to identify immediate neighbors of particles and it is one of the best adaptive methods to recover a precise density field from a discrete distribution of points, with clear advantage over Smoothed Particle Hydrodynamic or other interpolation based techniques (Schaap and van de Weygaert, 2000; Pelupessy et al., 2003), where its principal asset is its complete independence of arbitrary smoothing functions and parameters specifying the properties of these. VT reproduce the anisotropies of the local particle distribution and through its adaptive and local nature proves to be optimally suited for uncovering the full structural richness in the density distribution. Other remarkable uses of VT in this field are filamentary structure identification (González and Padilla, 2010) and N-body simulation code AREPO (Springel, 2010).

There are several serial open source VT implementations such as Qhull\(^1\) (Barber et al., 1996), or Voro++\(^2\) (Rycroft, 2009). There are also parallel algorithms for VT computation such as Starinshak et al. (2014), however none of them are open source and freely available to the community.

The purpose of this code is to be an open source tool for VT computation of large data sets, parallel and optimized to take full advantage of actual multicore and cluster architectures, user-friendly with documentation, and with typical I/O formats used in the field of N-body simulations. In addition, this code computes useful properties such as Voronoi density, cell volumes, and immediate neighbors lists.

2. Implementation

Code is developed in C, MPI and use re-entrant Qhull C library, and it is organized in different separated modules. A brief description of the code is shown in the flow diagram from figure, where code run sequentially from top to bottom, and parallelization is represented as horizontal branches.

After initialization, domain decomposition is defined depending on the number of tasks and configuration. There are two domain decomposition schemes, a) split he volume in power of 2 number of tasks with equal volumes, and balancing the cuts in all dimensions. Therefore, for \(N_{\text{task}}\), volume is split in each dimension by \(nx, ny, nz\) such as \(nx \times ny \times nz = N_{\text{task}}\). i.e.

\(^1\)http://www.qhull.org
\(^2\)http://math.lbl.gov/voro++
N_t = 32 split volume in each dimension by \( n_x = 4, \ n_y = 4, \) and \( n_z = 2. \) b) split the volume along a single direction \( N_t \) times. Scheme a) is most suitable for simulation boxes, and b) for irregular volumes such as survey slices.

Input file is read by a single root task, particles are read in blocks of a given buffer size, then each block is broadcast to the other Tasks. Each task select and allocate the particles from the buffer depending on domain decomposition.

After read and split particles in all tasks, each task define which particles should be sent to neighbors task as boundary particles. The thickness of the layer of boundary particles is defined in terms of inter-particle distance and can be configured in the code, this value should be at least larger than 1.0, however if this value is too large, we will have an excess of unnecessary boundary particles. In figure 2 we show a graphical example why boundary particles are needed when we split particles in several sub-volumes according domain decomposition. Top panel show a particle distribution in 2D which
will be split by the vertical black line, then middle panel show how the VT of particles at the border of division fail if no boundary consideration are taken(red lines), so in bottom panel we add some boundary particles(red dots), then failed particles from middle panel (grey dashed) now have a correct VT.

Figure 2: Consistent treatment of task boundaries. Top panel) an example particle distribution in 2D with their corresponding VT. We want to split particles in two processes defined by the vertical black line. Middle panel) If we compute VT of particles at the right side, particles at the border of division will have an incorrect VT computation, see red lines. Bottom panel) if we add boundary particles(Red dots), the VT of previously mentioned particles(gray dashed) will have a correct VT.

The next step, after all boundary particles are transferred is VT computation using Qhull library in each task, then for each particle the code
look for all their facets to compute Voronoi cell volume. Therefore, density is computed using particle mass and Voronoi cell volume. In addition, the code follow Voronoi facet structure to identify all neighbors for each particle. Optionally, the code compute average Voronoi density in a regular grid, where each task resolve its corresponding region of the total grid.

After all task finishes computation, each task send back to root task output information (density, volume, neighbors) in blocks, root task re-index particles of each block based on input file order, and re-index VT neighbor information aswell by replacing boundary particles indices by real particles indices, and write output files in blocks, after all blocks are transmitted. In figure 3, we show VT structure output of a small galaxy distribution produced by this code.

3. Performance

The nice part of VT parallelization is that computation is very local and for a given particle, its VT depends only on its neighbors, and no long range computations are required. When we split the volume in different tasks, even if we add an overhead of boundary particles, total computation time is strongly reduced.

We have Qhull runs VT in $O(N_P \log N_V)$ for a typical 3d particle distribution, where $N_P$ is the number of particles, and $N_V$ is the number of vertices. In typical cosmological simulation the number of vertices is $\sim 7 - 10$ times $N_P$ depending on particle distribution and clustering. Then scaling should be close to linear.

We run performance tests in two nodes with following specifications:

SuperServer 2U 8028B-COR3FT - Dual Socket R (LGA 2011)
4 INTEL HASWELL-EX 14C E7-4850V3 2.2G 35M 8GT/s
32 16GB DDR3-1600 1.35V 2Rx4 ECC REG DIMM
Mellanox ConnectX-3 VPI, QSFP QDR IB (40Gb/s) and 10GbE

In figure 4, we show scaling of the code for two cosmological Nbody dataset, where boundary thickness is defined as 1.5 times the inter-particle distance. A small test with $\sim 3.5$M particles, and a medium test with $\sim 27.5$M particles. Computation times are normalized per million particles. We have in both test cases scaling is almost linear, and differences from linear case
Figure 3: VT structure of a mock galaxy distribution.
Figure 4: Time benchmarks per million particles as function of the number of tasks for: a small test of \(\sim 3.5\) Million particles (blue), and a medium test of \(\sim 27.5\) Million particles (red). Dashed lines just represent a linear scaling progression. Computation times exclude I/O operations.

appears at larger number of tasks since we add more communication and synchronization between tasks, and the number of boundary particles increases as well.

Parallelization speedup degrades dramatically when the number of boundary particles becomes similar to the number of input particles, and it depends
on particle distribution. A safe limit for parallelization is when boundary particles are lower than 20% input particles, this can be regulated by the number of tasks and setting the boundary layer thickness.

Code consumes around $\sim 3$Gb of ram per million particles, this can be halved changing code parameters at the cost of performance and precision.

3.1. Discussion

PARAVT is a new parallel and open source code for VT computation designed to handle large number of particles, it is focused for astrophysics purposes with I/O formats compatible with common Nbody processing tools. Additional properties are computed for each particle, such as Voronoi density, cell volumes and neighbors list.

Key features of this code are:

- MPI parallel code which makes possible VT computation of large data-sets taking advantage of multicore and cluster architectures.
- VT of particles at boundaries of tasks sub-volumes are properly computed and neighbors re-indexed as a single volume.
- Computes neighbors list for each particle.
- Computes Voronoi density and cell volumes for each particle.
- Optionally can computes average density on a regular grid.
- Periodic conditions and multimass particles.
- ASCII and Binary I/O format.
- Gadget and Rockstar input formats, specially for N-body cosmological analysis.
- Raw Qhull output, memory and precision management, VTK grid output for quick visualization.
- User guide.

Check repository: https://github.com/regonzar/paravt
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References


