



# High-Performance Computation of Distributed Memory Parallel 3D Voronoi and Delaunay Tessellation

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# Executive Summary

We developed a prototype library for computing in situ Voronoi and Delaunay tessellations from particle data and applied it to cosmology, molecular dynamics, and plasma fusion.

## Key Ideas

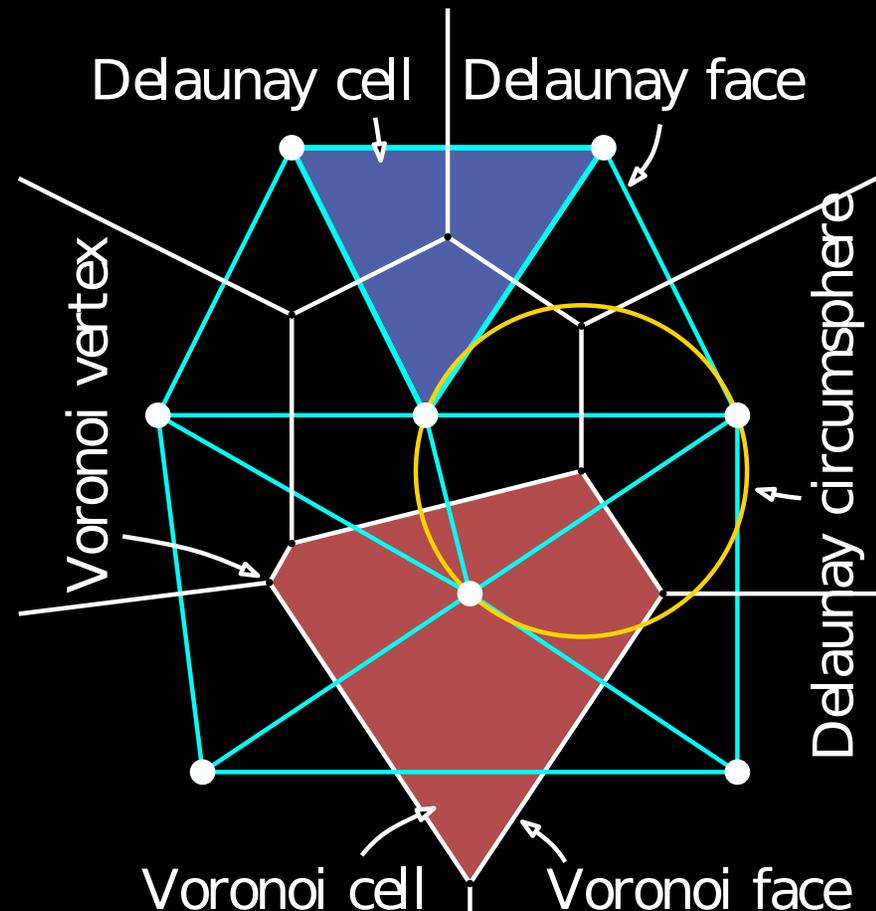
- Mesh tessellations convert sparse point data into continuous dense field data.
- Meshing output of simulations is data-intensive and requires supercomputing resources
- No large-scale data-parallel tessellation tools exist.
- We developed such a library, tess.
- Features:
  - Automatic neighbor point determination (simple local protocol)
  - Periodic and wall boundary conditions
  - Good parallel performance and scalability.
  - Widespread applicability in addition to the datasets we tested.

# Computational Geometry 101

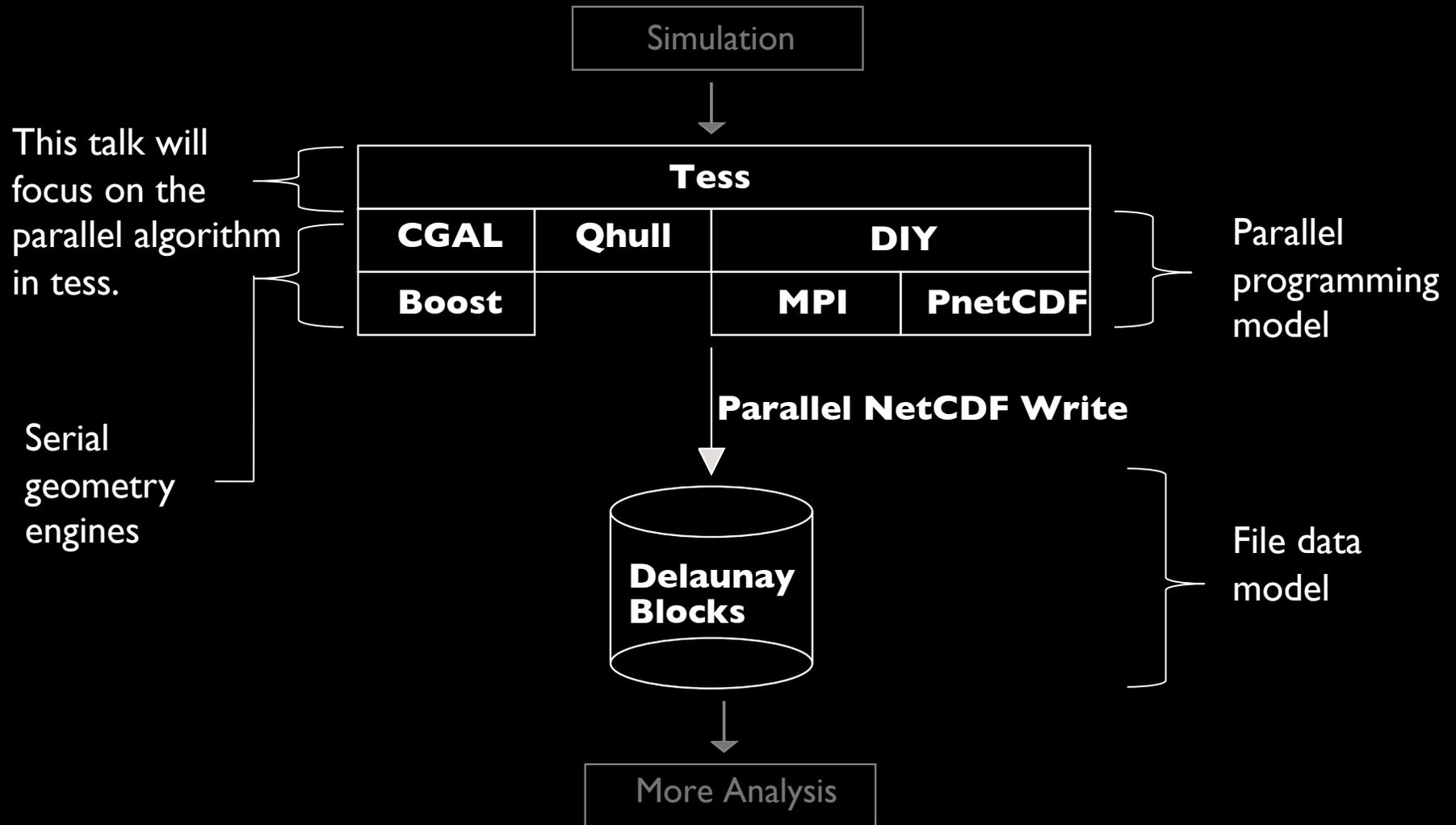
The diagram is drawn in 2D for simplicity, but all our work is in 3D: polygons in the figure correspond to polyhedra and triangles to tetrahedra.

## Terms

- Input points (3D)
- Voronoi cells (polyhedra)
- Delaunay cells (tetrahedra)
- Delaunay, Voronoi faces
- Voronoi vertices
- Delaunay vertices = input points
- Delaunay circumpheres (empty of input points)
- Duality: Voronoi vertex = center of Delaunay circumphere, Voronoi face  $\leftrightarrow$  Delaunay edge



# Software Structure

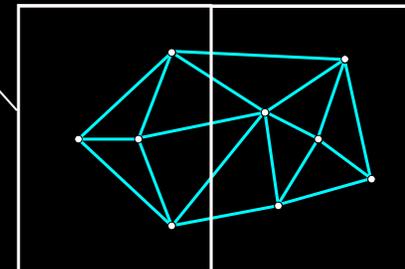
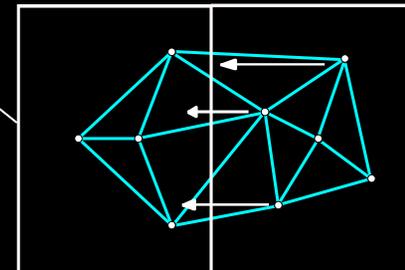
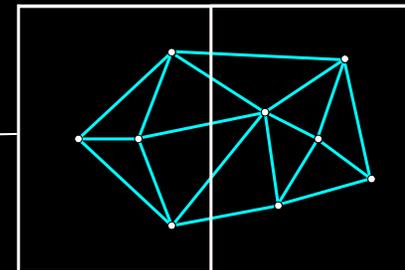
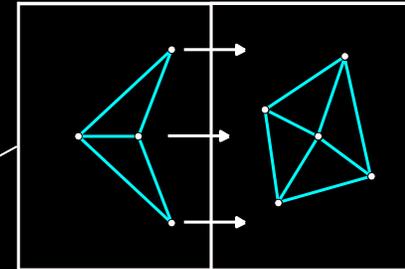
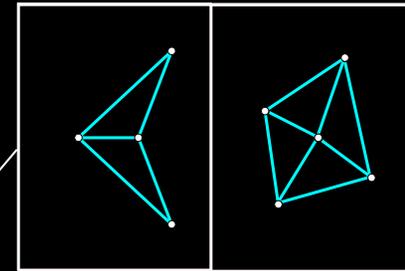


# Overall Algorithm

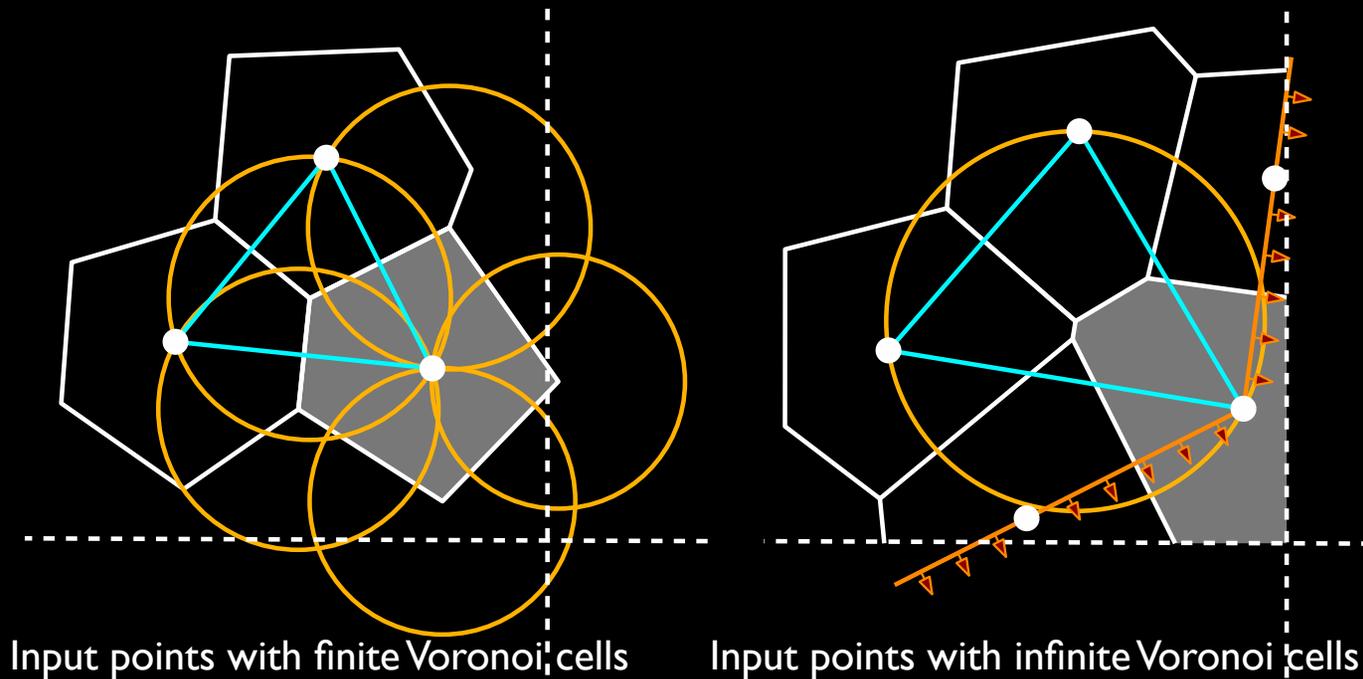
1. Compute initial local tessellation
2. Exchange initial neighbor points
3. Compute augmented local tessellation
4. Exchange remaining neighbor points
5. Compute final local tessellation
6. Write tessellation to storage

## Fine Print

- No tetrahedron is larger than a 1-neighborhood of blocks
- Implementation detail, not a fundamental limitation



# Neighbor Point Exchange



## Pass 1:

Send finite cell points to neighbors within circumsphere

Send infinite cell points to single closest neighbor

Compute new tessellation

## Pass 2:

Send finite cell points that were infinite in Pass 1 to neighbors within circumsphere

Send remaining infinite cell points to all neighbors

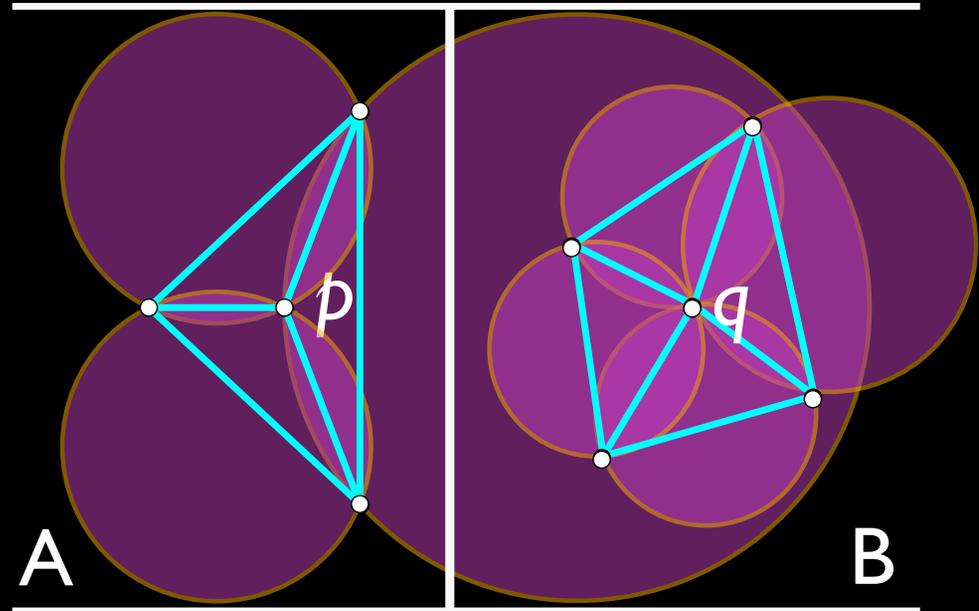
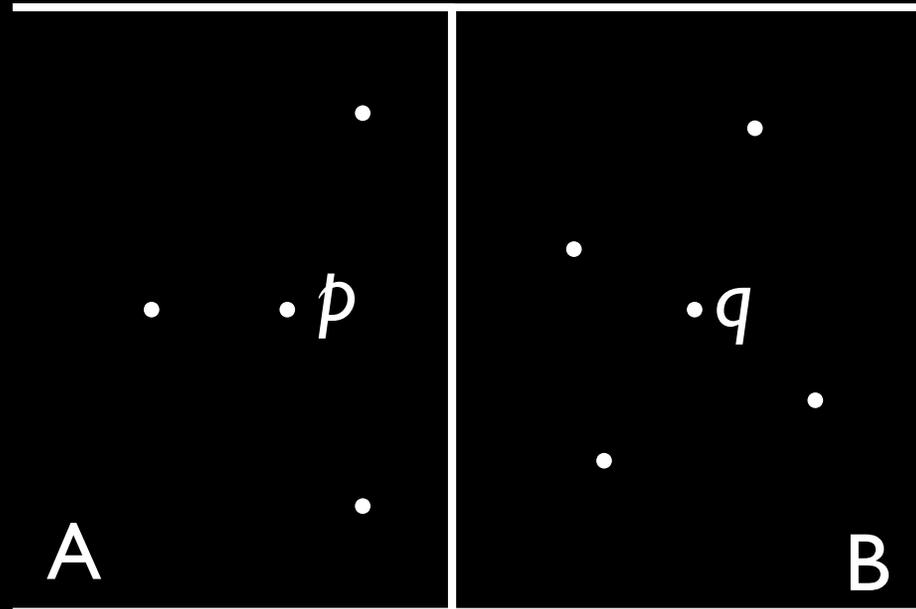
# Points with Finite Voronoi Cells: Local Determination of Neighbor Point Communication

## 3 Rules

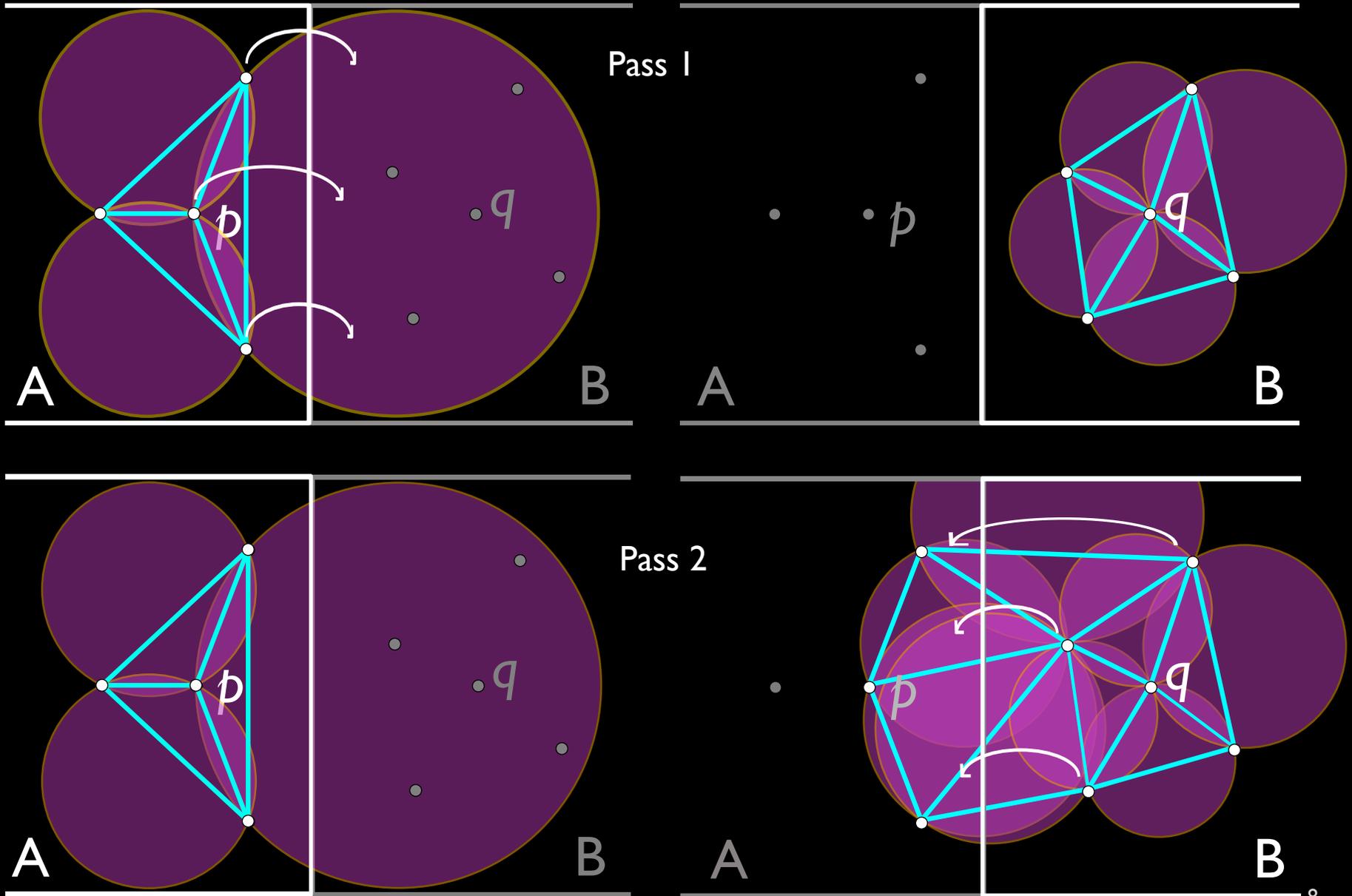
- Send any point lying on a circumsphere that intersects a neighbor to that neighbor.
- Don't send a point to the same neighbor twice.
- Don't send a non-original point (point received from a neighbor).

## Benefit

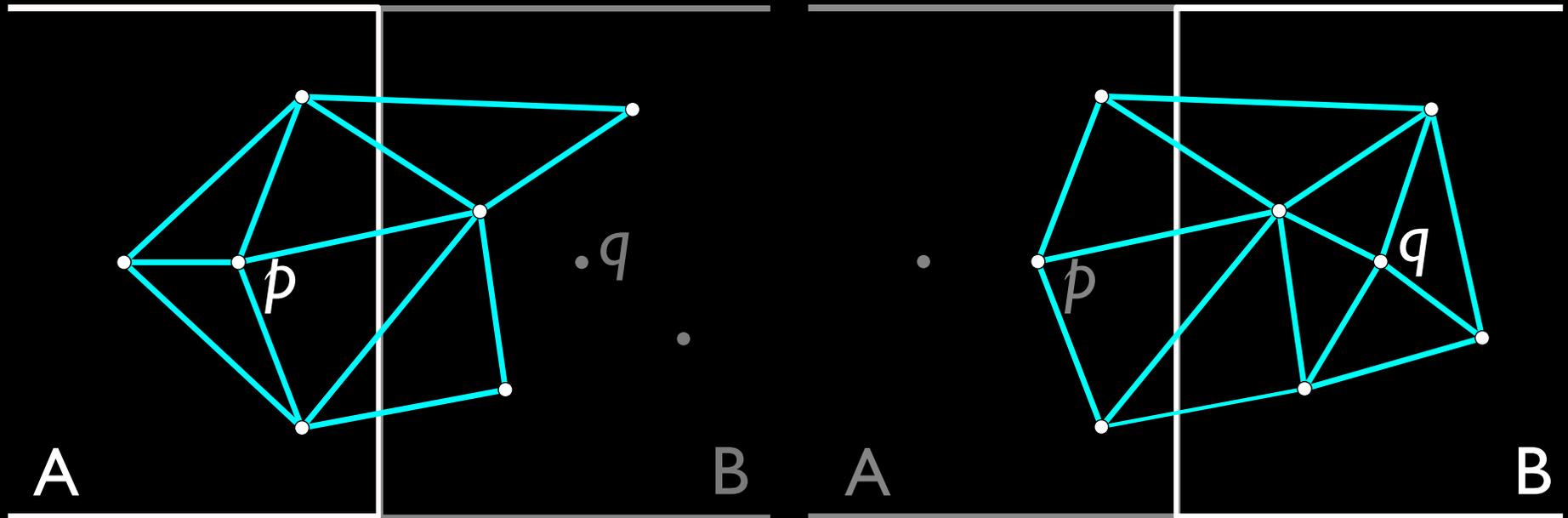
- Sending is determined locally
- Never have to ask a neighbor in order to send or receive



# Points with Finite Voronoi Cells: 2 Passes



## Points with Finite Voronoi Cells: Final Result



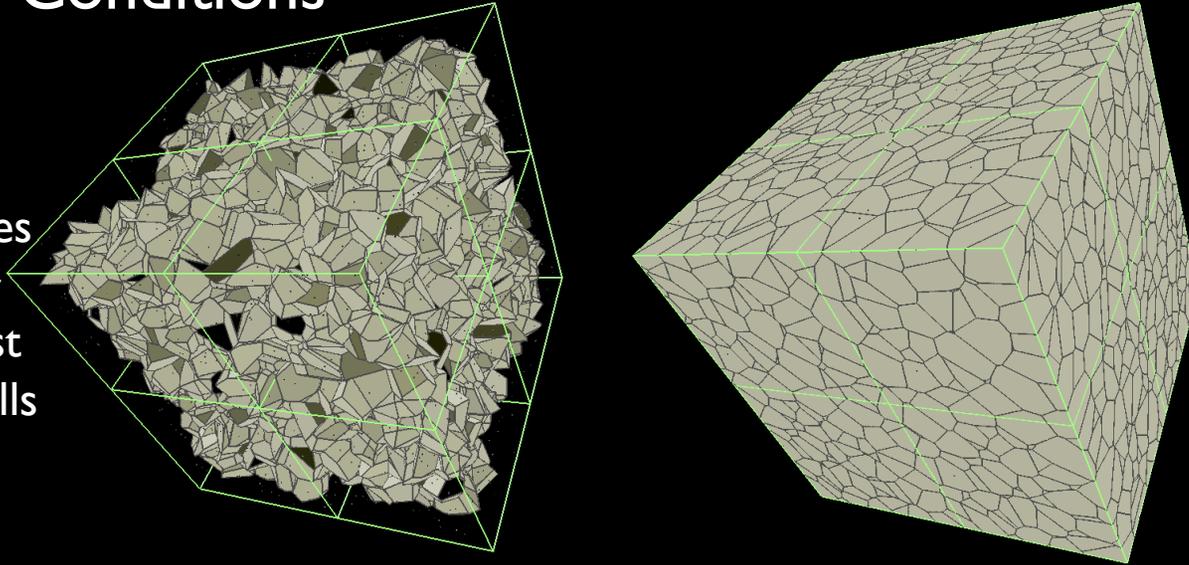
Each block has all the information it needs to construct complete Delaunay tetrahedra and Voronoi cells

- Some particles are duplicated: block owning the original particle is the “true” owner.
- Some tetrahedra are duplicated: of the blocks owning the 4 vertices, the block with the minimum global block ID # is the “true” owner.

Functions are included to traverse the Delaunay tessellation and construct the Voronoi tessellation on the fly.

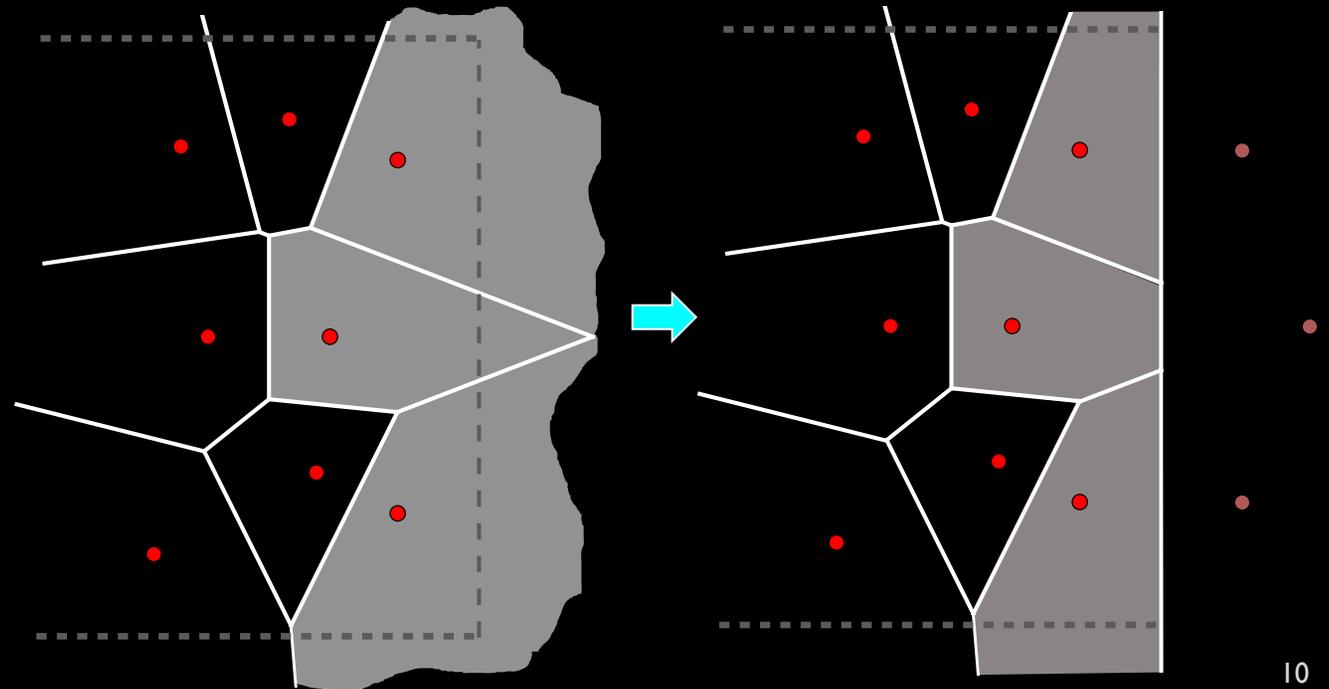
# Wall Boundary Conditions

Wall boundary conditions occur in simulations of particles packed in a container or sedimenting against a surface. Voronoi cells intersecting a wall should be clipped to the wall.

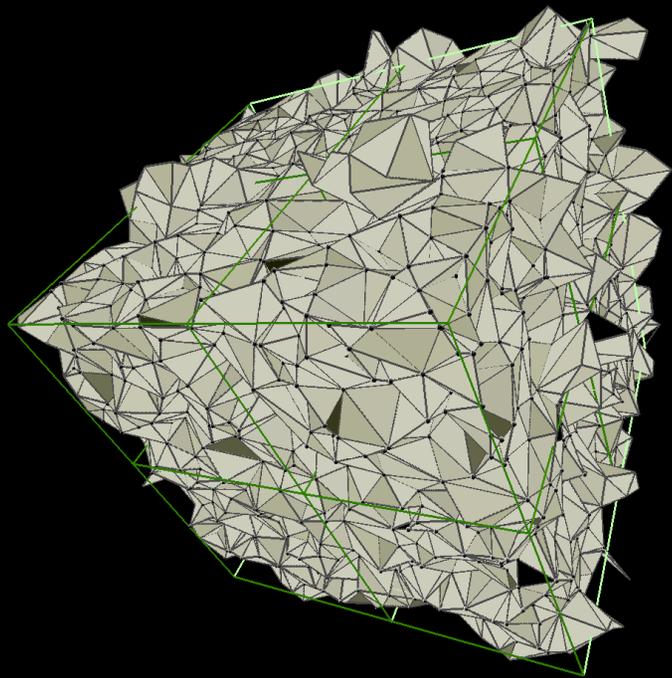


To apply a planar wall boundary condition, we add a “virtual” point that is the mirror image of the point across the wall.

The Voronoi definition guarantees that the cell face will conform to the wall.

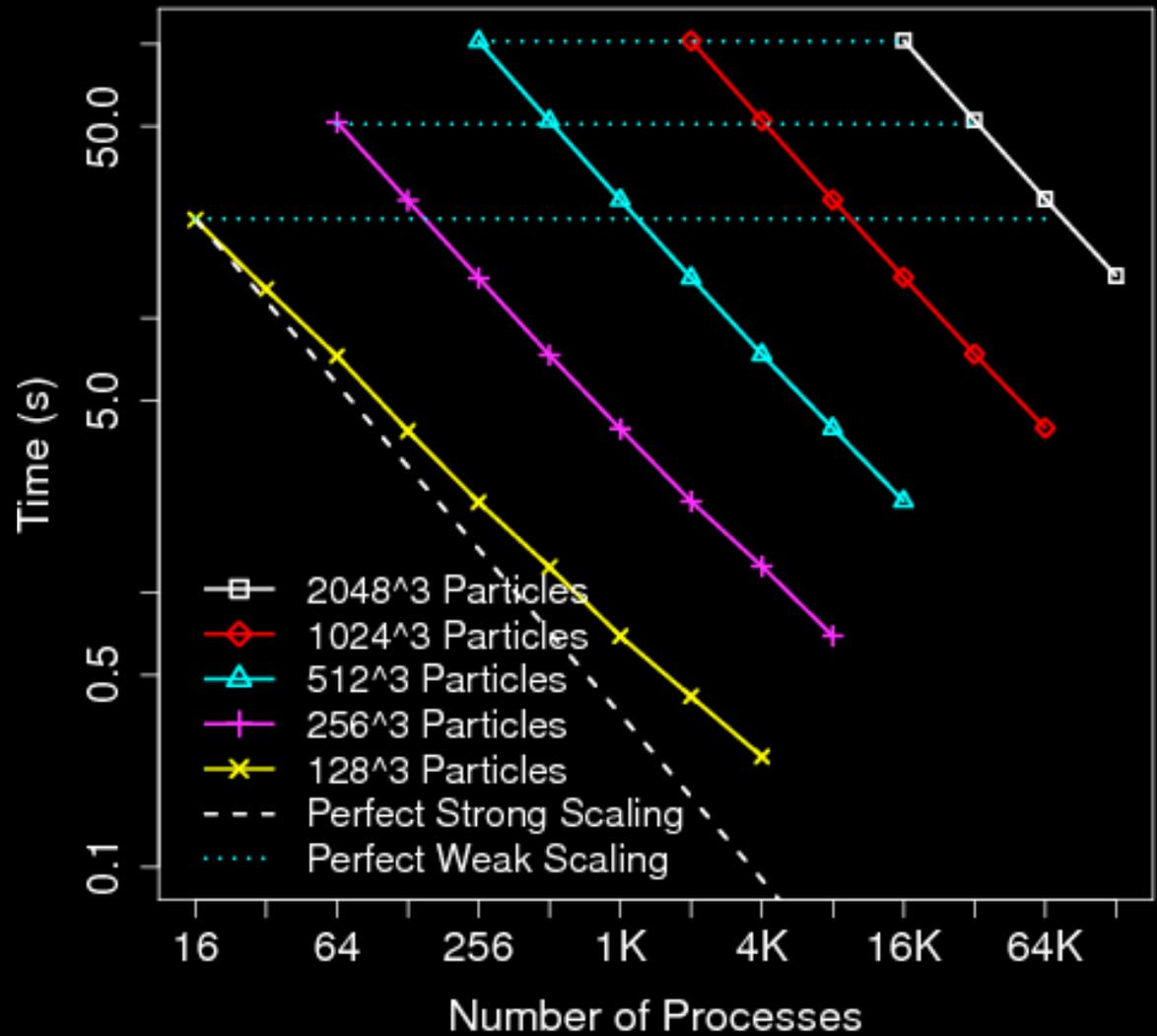


# Scalability



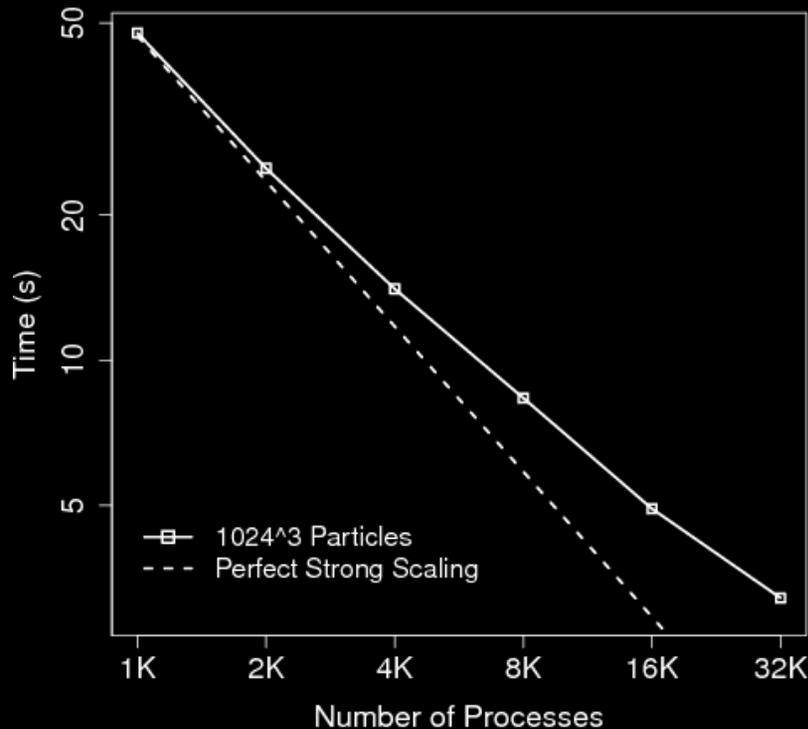
Strong and weak scaling for up to  $2048^3$  synthetic particles and up to 128K processes (excluding I/O) shows up to 90% strong scaling and up to 98% weak scaling.

## Strong and Weak Scaling with CGAL

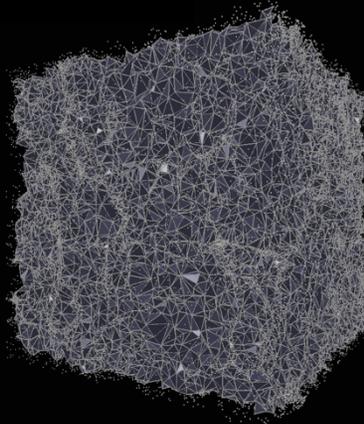


# More Performance and Scalability

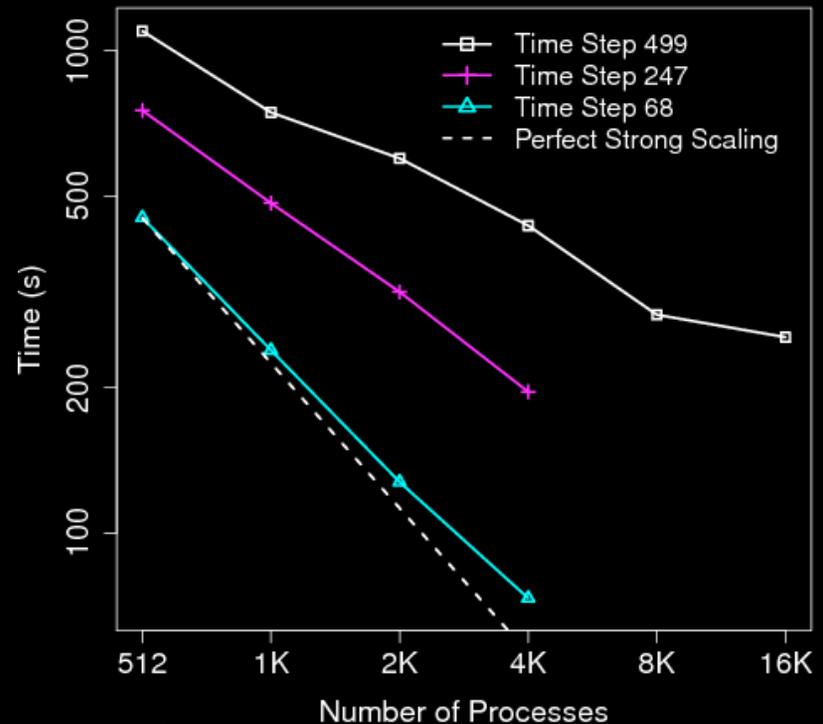
Strong Scaling of Nyx Data on Edison



Strong scaling (excluding I/O time) using CGAL for a Nyx middle time step of  $1024^3$  particles. The load imbalance at this time step is not as severe as in the HACC example at the right; strong scaling efficiency is 46%.

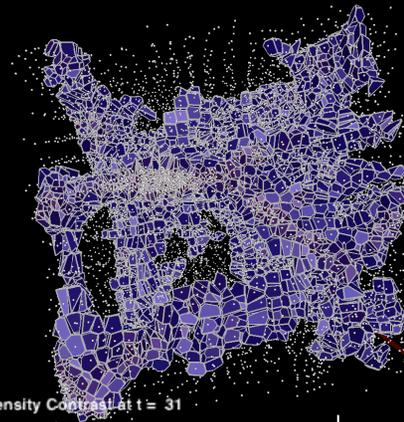


Strong Scaling of HACC Data on Mira



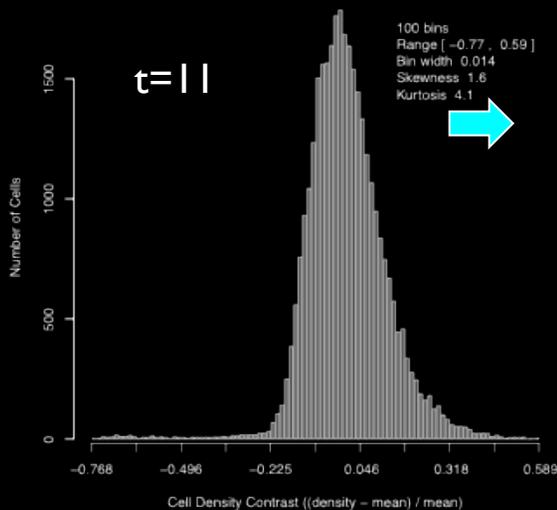
Strong scaling (excluding I/O time) using CGAL for three time steps of HACC data of  $1024^3$  particles. At later time steps, particles cluster into extremely dense and sparse regions, affecting load balance and reducing efficiency from 77% at  $t=68$  to 14% at  $t = 499$ .

# Applications in Cosmology

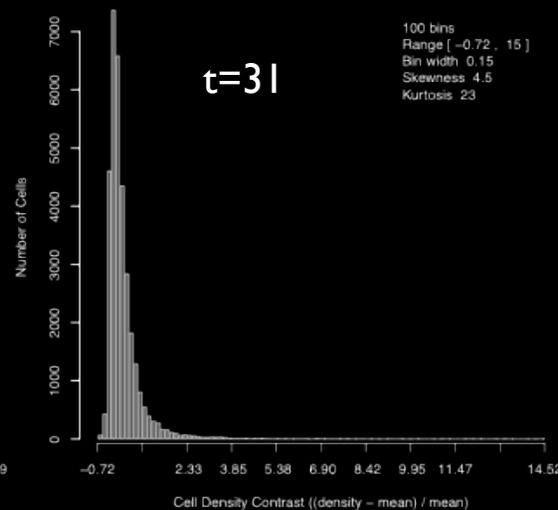


Feature statistics: Total volume, surface area, curvature, topology of connected components of Voronoi cells classify and quantify features.

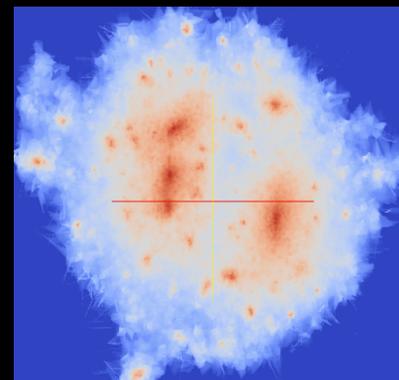
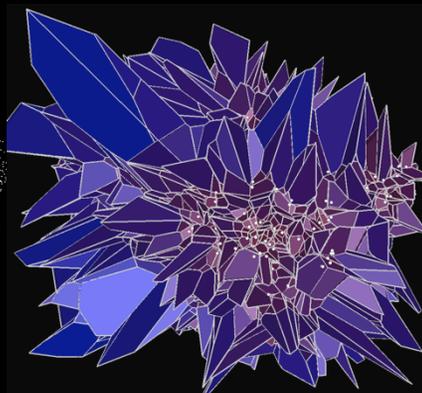
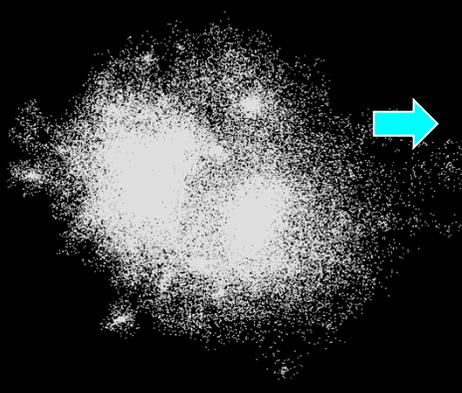
Histogram of Cell Density Contrast at  $t = 11$



Histogram of Cell Density Contrast at  $t = 31$



Temporal dynamics: Over time, the range of Voronoi volume, kurtosis, and skewness increases, consistent with the governing physics of the formation of high- and low-density structures in the universe.

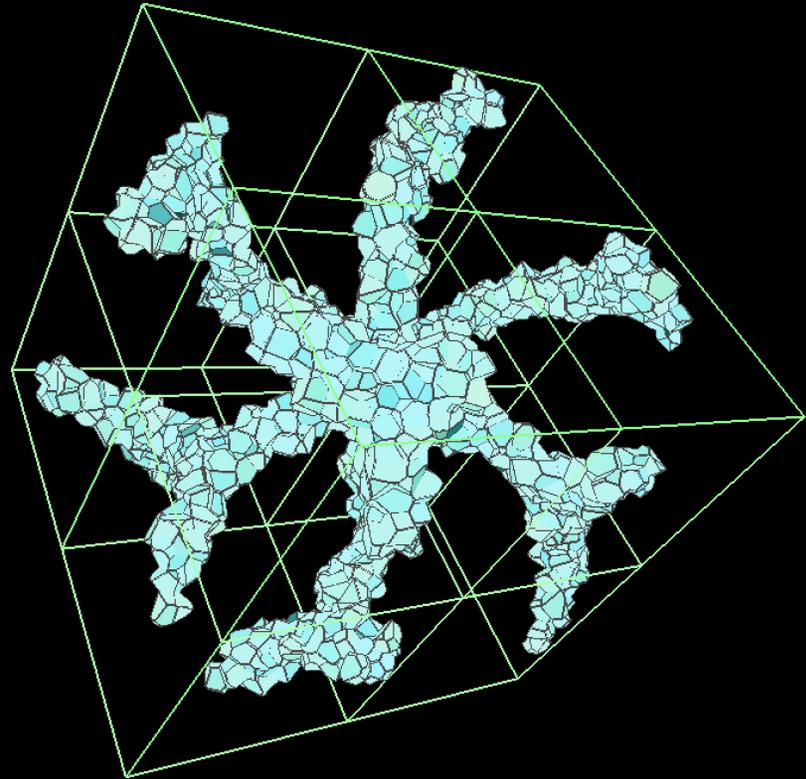


Density estimation: Tessellations as intermediate representations enable accurate regular grid density estimators.

# Applications in Molecular Dynamics

In simulations of soft matter systems, populations of molecules self-organize to form two or more species. These domains can form complicated geometries such as the double gyroid.

Voronoi tessellation of 1,000 A-B-C “telechelics” composed of two nanospheres (A and C) connected by a polymer tether beads (B) for a total of 8,000 beads in a double gyroid morphology. Only the Voronoi cells associated with the A species are shown.



We tessellated over 300 time steps of an A-B-A triblock copolymer (176,960 total beads) found in an alternating gyroid morphology. Summing the Voronoi cells of the A and B species suggests that because the B part has to stretch or fold, the B domain dilates relative to the A domain.

# Wrapping Up

We developed a prototype library for computing in situ Voronoi and Delaunay tessellations from particle data and applied it to cosmology, molecular dynamics, and plasma fusion.

## Contributions

- Automatic neighbor point determination (simple local protocol)
- Periodic and wall boundary conditions
- Good parallel performance and scalability.
- Widespread applicability in addition to the datasets we tested.

## Ongoing, Future

- Open source licensing
- KD tree for load balancing
- Hybrid distributed/shared memory implementation (MPI + threads)

“The purpose of computing is insight, not numbers.”

–Richard Hamming, 1962

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