Computational geometry of soft matter

UMass Summer School on Soft Solids and Complex Fluids 2024
Lecture 2 (Tuesday June 4)

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Outline

Monday

- A model of dense granular drainage
- Voronoi analysis of granular flow
- Neighbor relations

Tuesday

- Development of the Voro++ library
- Network analysis for CO_2 capture
- Alternative models and methods

Wednesday

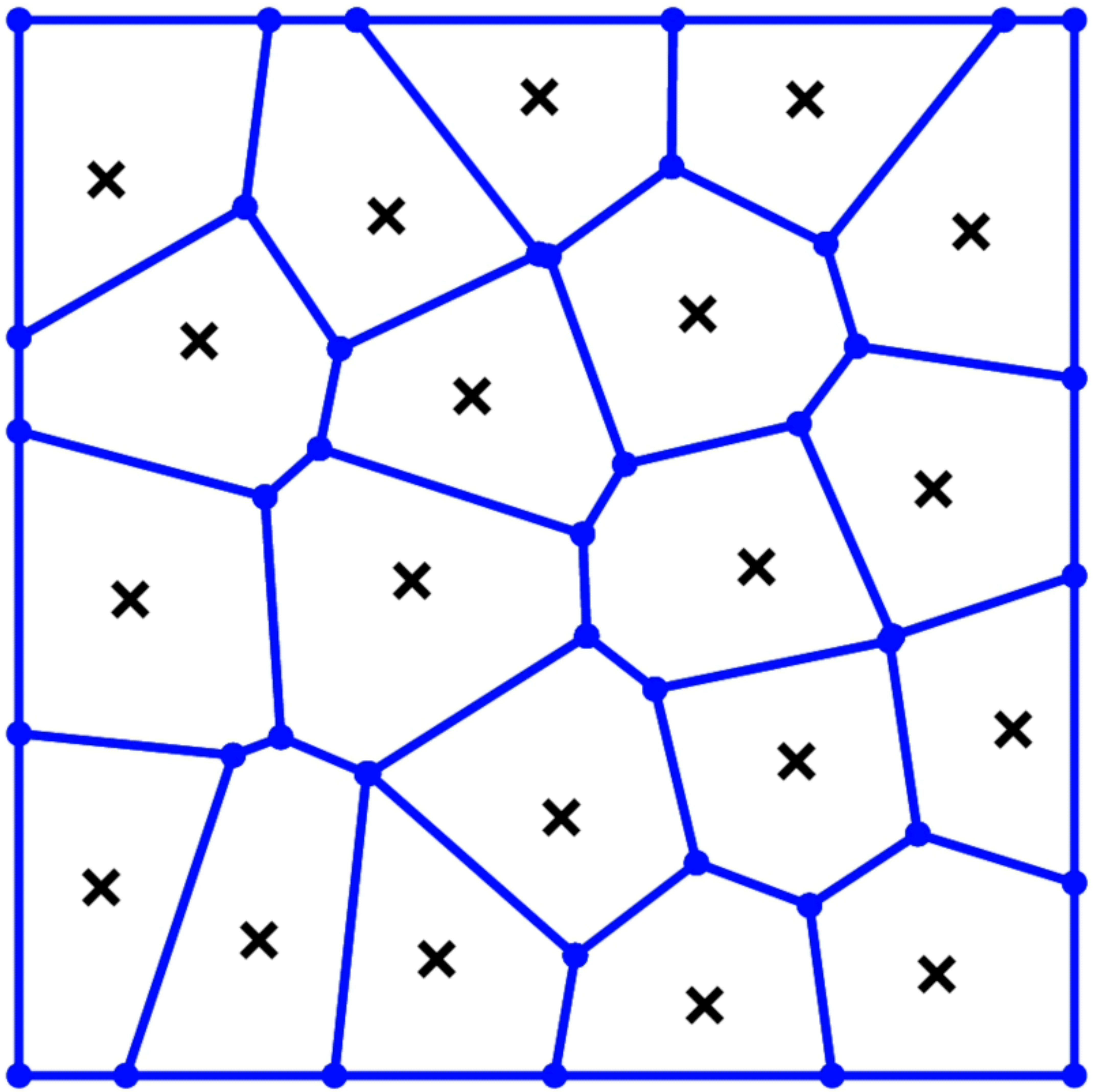
- Topological Voronoi analysis
- Lloyd's algorithm and meshing
- Insect wing structure

Thursday

- Continuum representations of deformation
- The reference map technique
- Fluid–structure interaction

Calculating an individual Voronoi cell

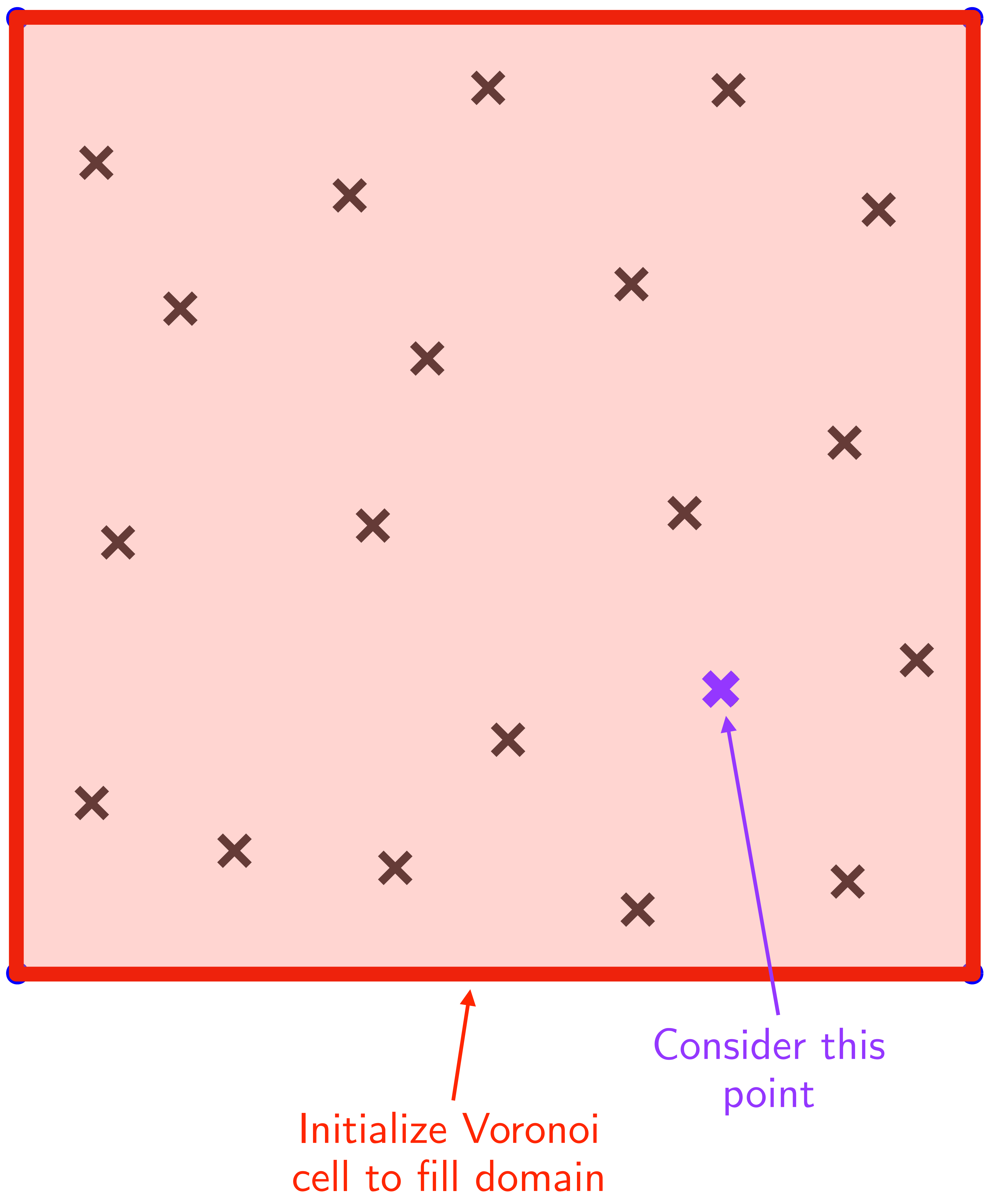
- There are a number of algorithms for computing the Voronoi tessellation:
  - **Incremental approach**: add particles one-by-one and recompute the vertices each time
  - **Fortune's sweeping algorithm**: builds the tessellation by sweeping an advancing front across the domain
  - **Quickhull algorithm:** finding the tessellation in $\mathbb{R}^n$ can be converted into computing a convex hull in $\mathbb{R}^{n+1}$; used by the *Qhull* software package



P. J. Green and R. Sibson, *Computing Dirichlet tessellations in the plane*, The Computer Journal **22**, 168–173 (1978).
S. Fortune, *A sweepline algorithm for Voronoi diagrams*, Algorithmica **2**, 153–174 (1987).
C. B. Barber *et al.*, *The quickhull algorithm for convex hulls*, ACM Trans. Math. Softw. **22**, 469–483 (1996).

Calculating an individual Voronoi cell

- An alternative method is to compute each Voronoi cell separately
- Initialize Voronoi cell to fill Ω
- Each neighboring particle cuts the Voronoi cell by a plane that is a perpendicular bisector
- After enough nearby particles are considered, the Voronoi cell is complete



A. Okabe *et al.*, *Spatial tessellations: Concepts and Applications of Voronoi Diagrams*, Wiley, 2000.
E. A. Lazar *et al.*, *Voronoi cell analysis: the shapes of particle systems*, Am. J. Phys. **90**, 469 (2022).

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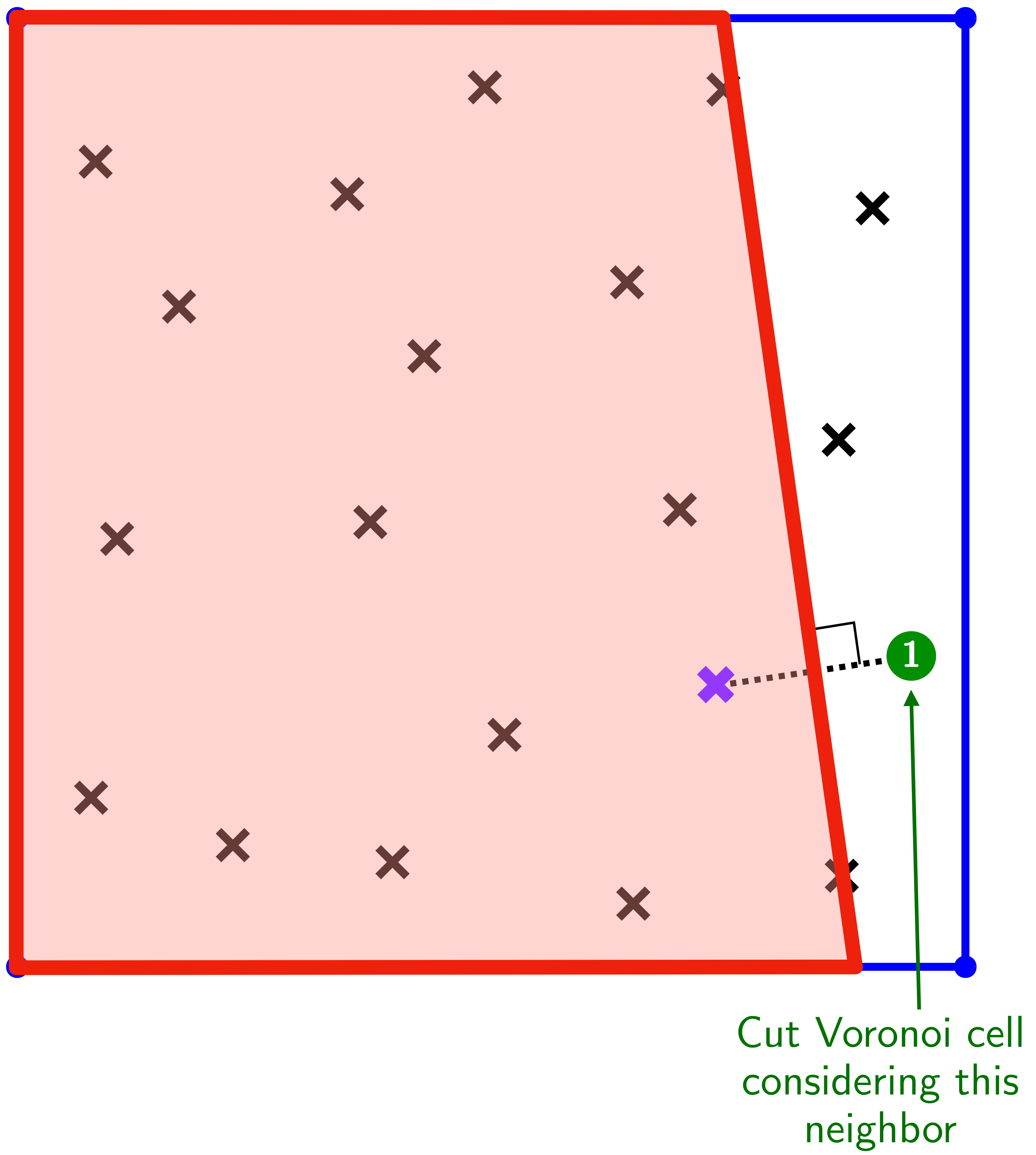

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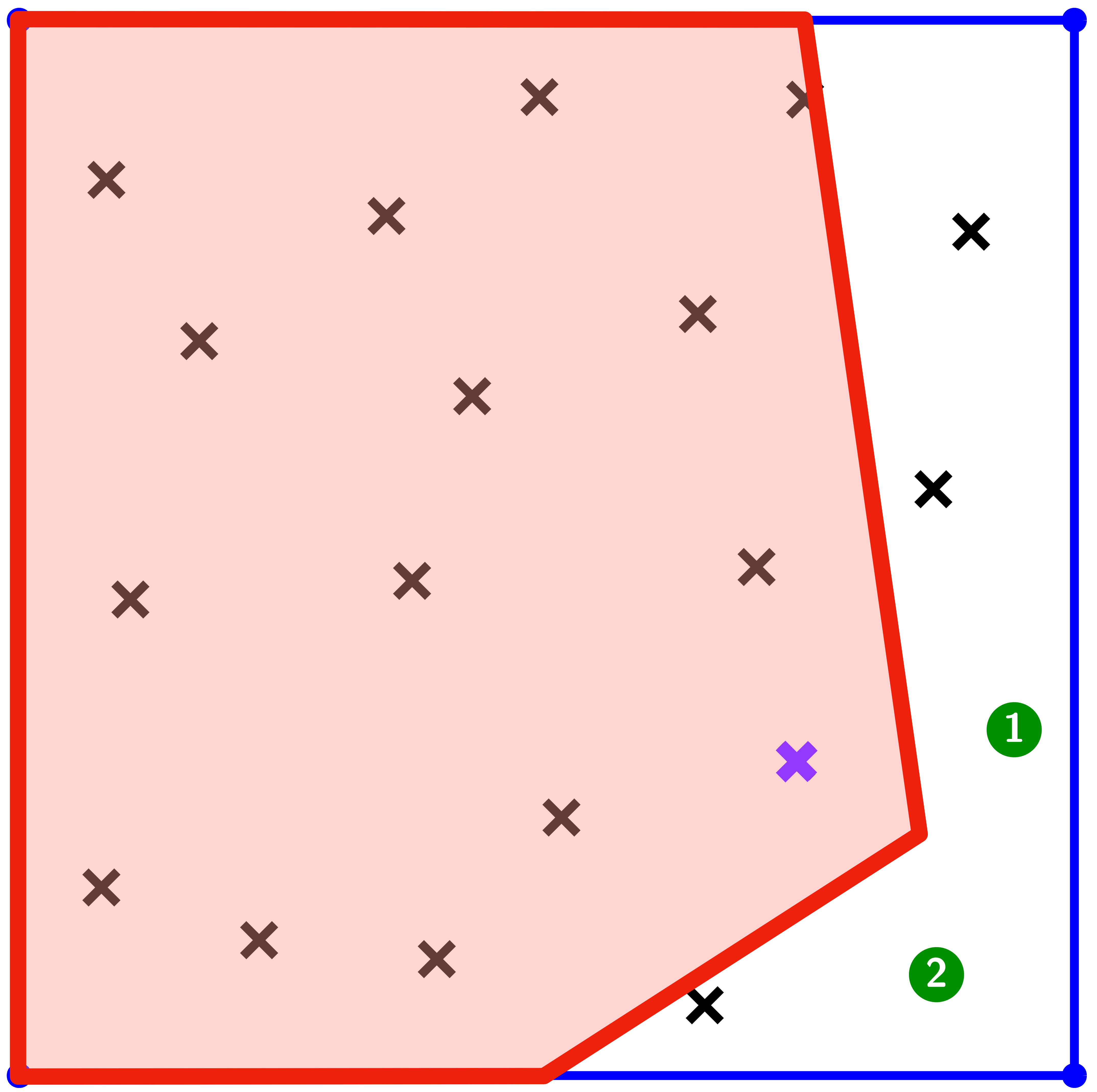

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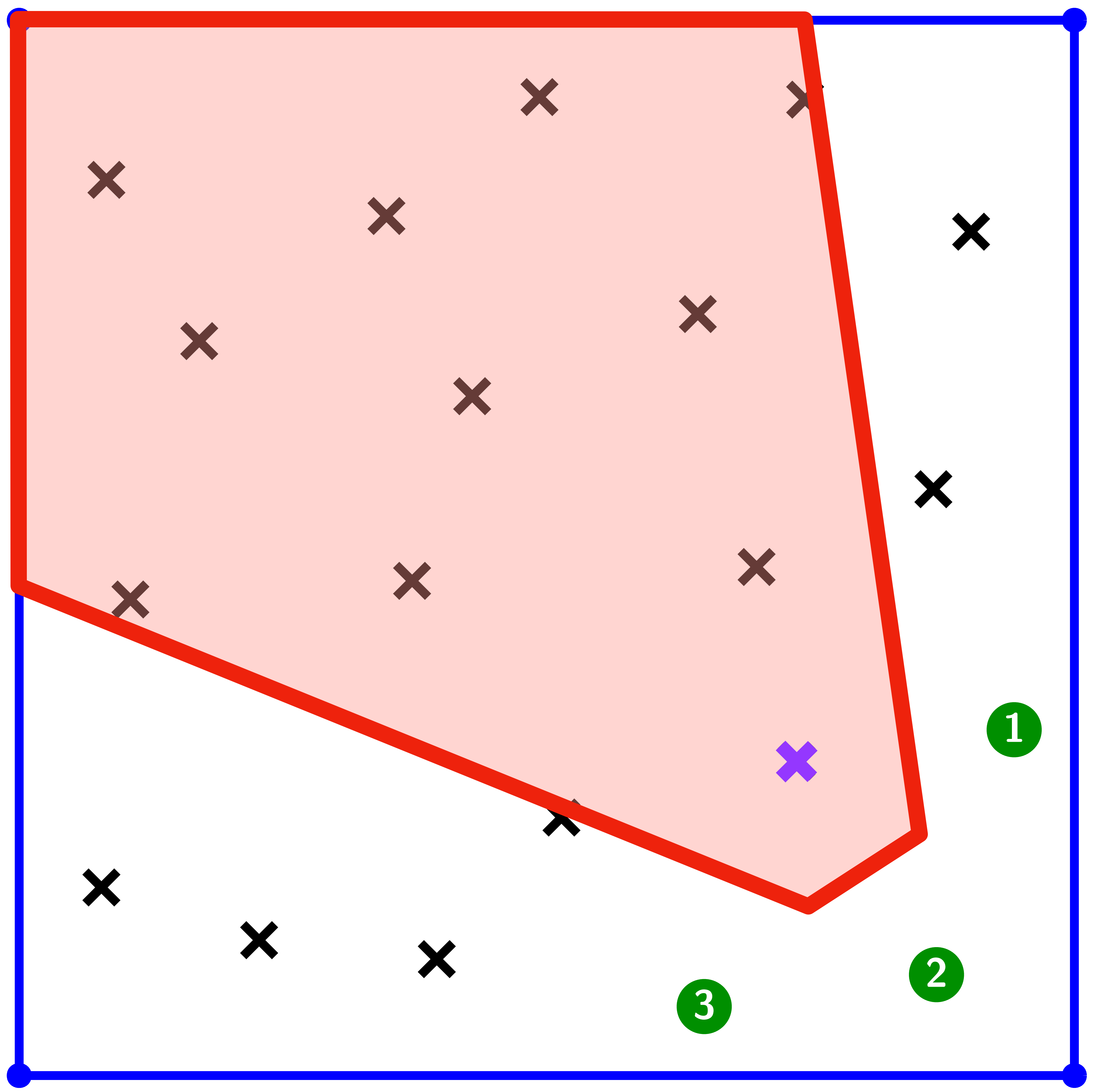

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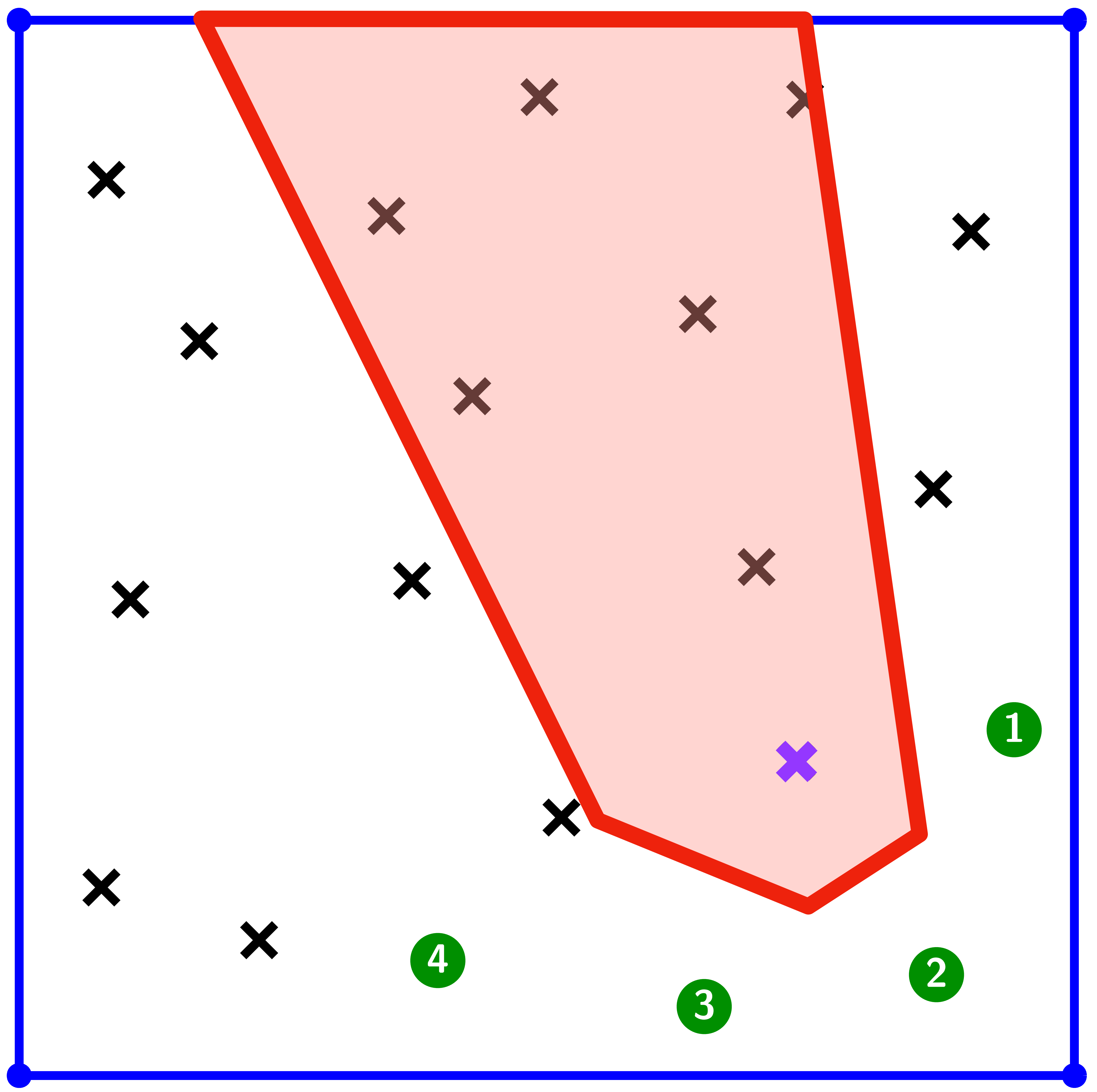

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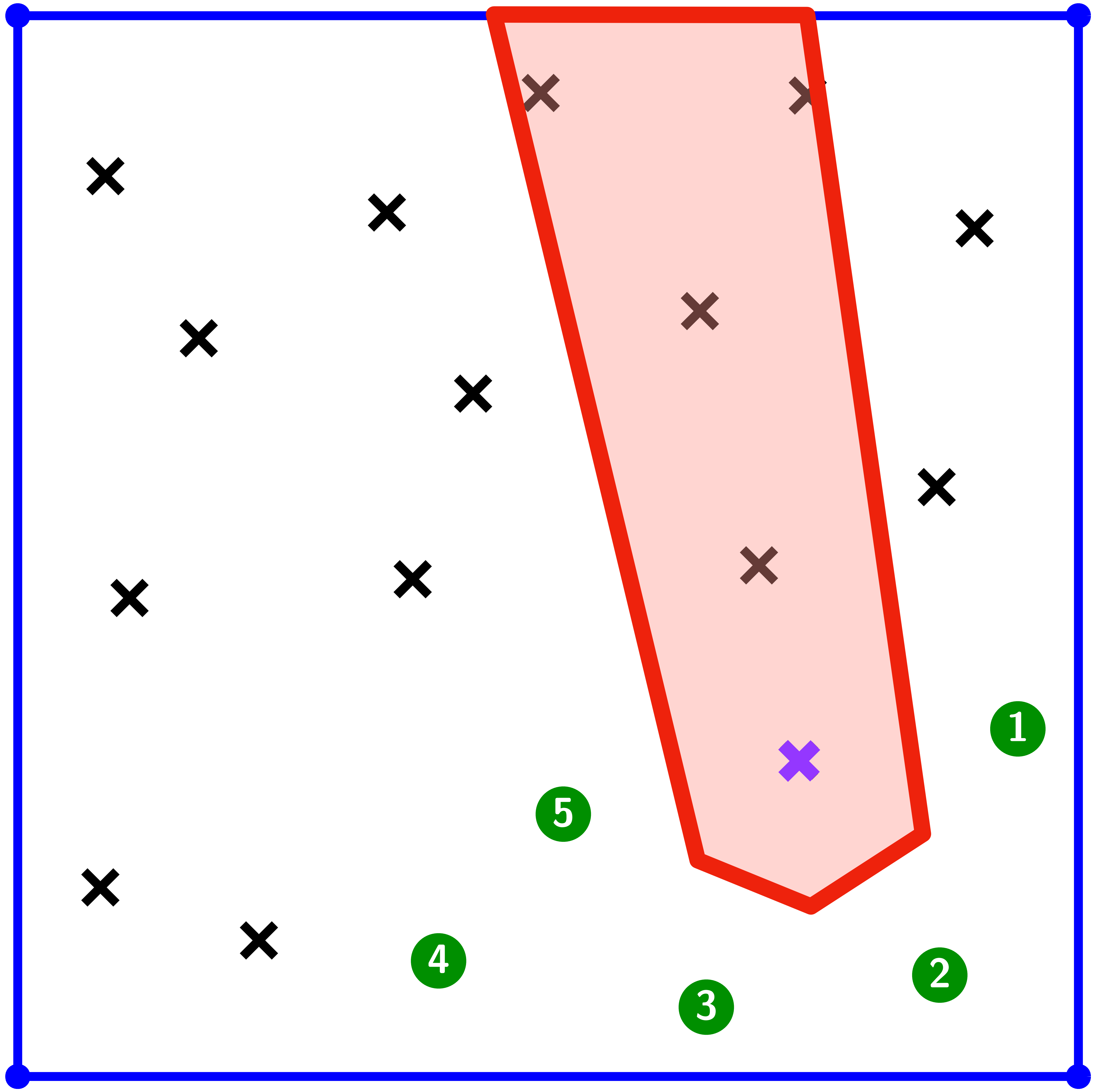

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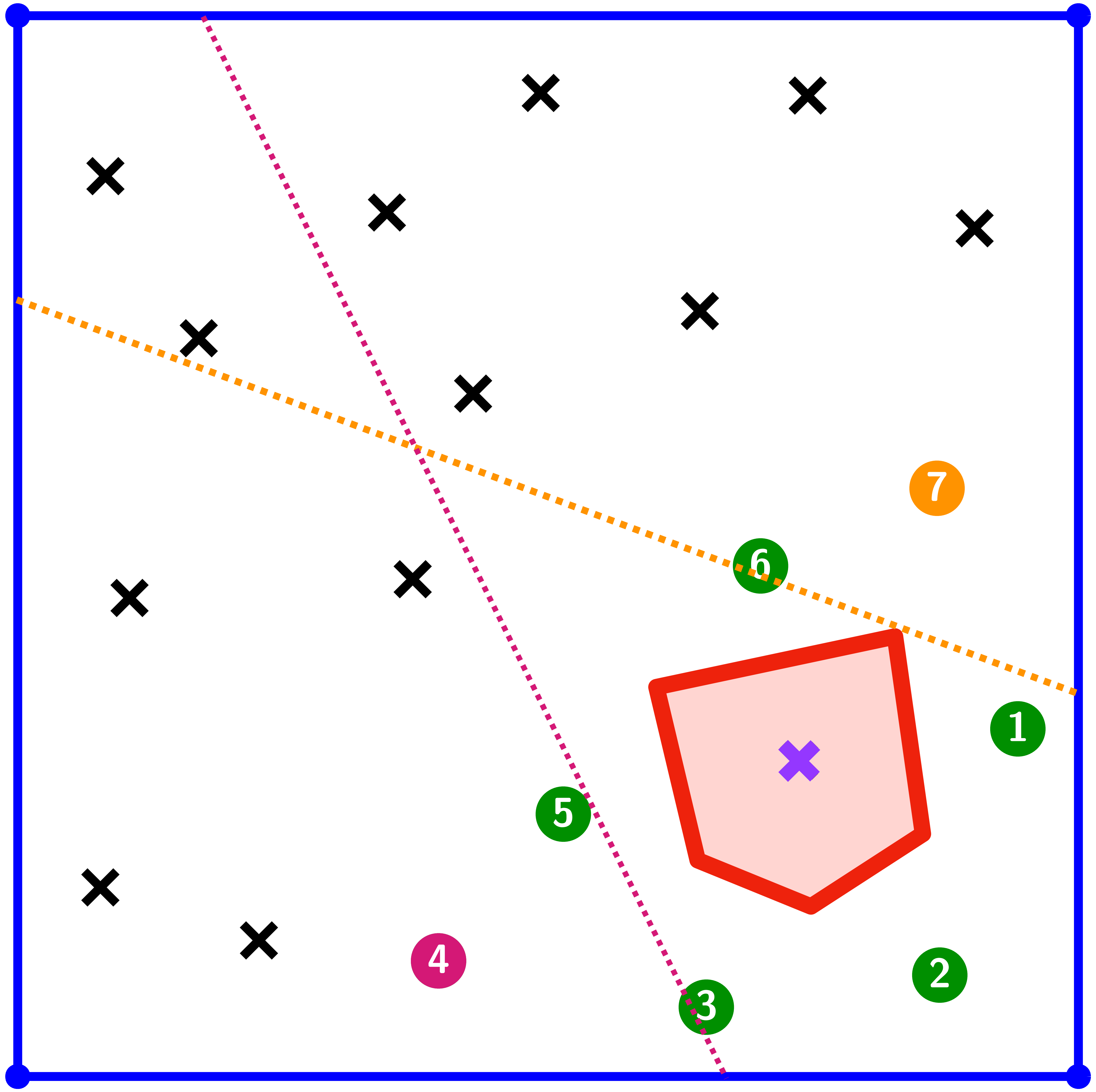

7 : considered, but didn't cut cell
4 : cut cell, but ultimately not needed
1,2,3,5,6 : required

A. Okabe *et al.*, *Spatial tessellations: Concepts and Applications of Voronoi Diagrams*, Wiley, 2000.
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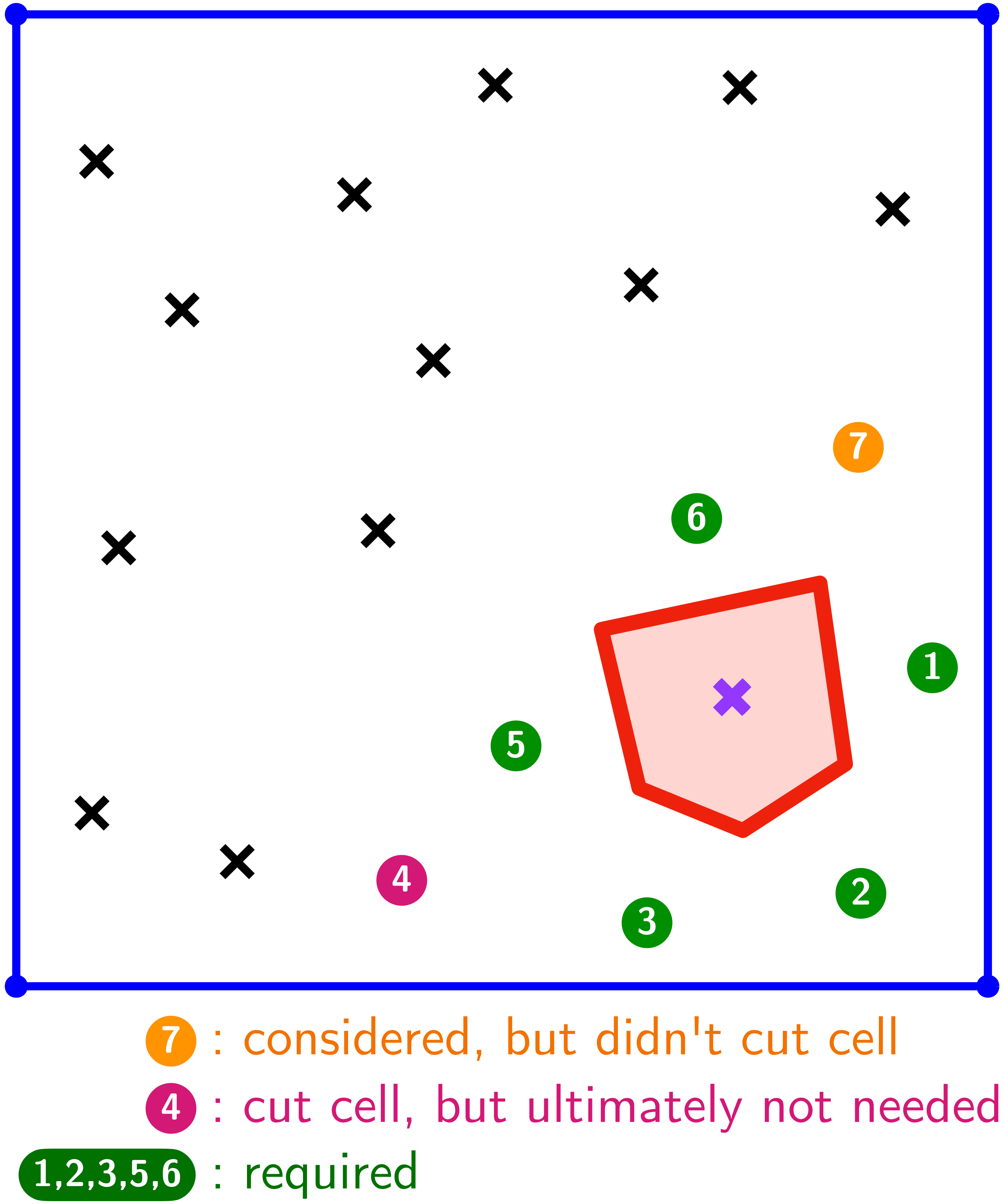
Computational considerations

- Each cell can be computed independently; has advantages for parallel computation
- The algorithm needs to consider nearby particles efficiently—we want to find the green particles, and minimize choosing orange/magenta particles
- The algorithm has some drawbacks—we will return to this later



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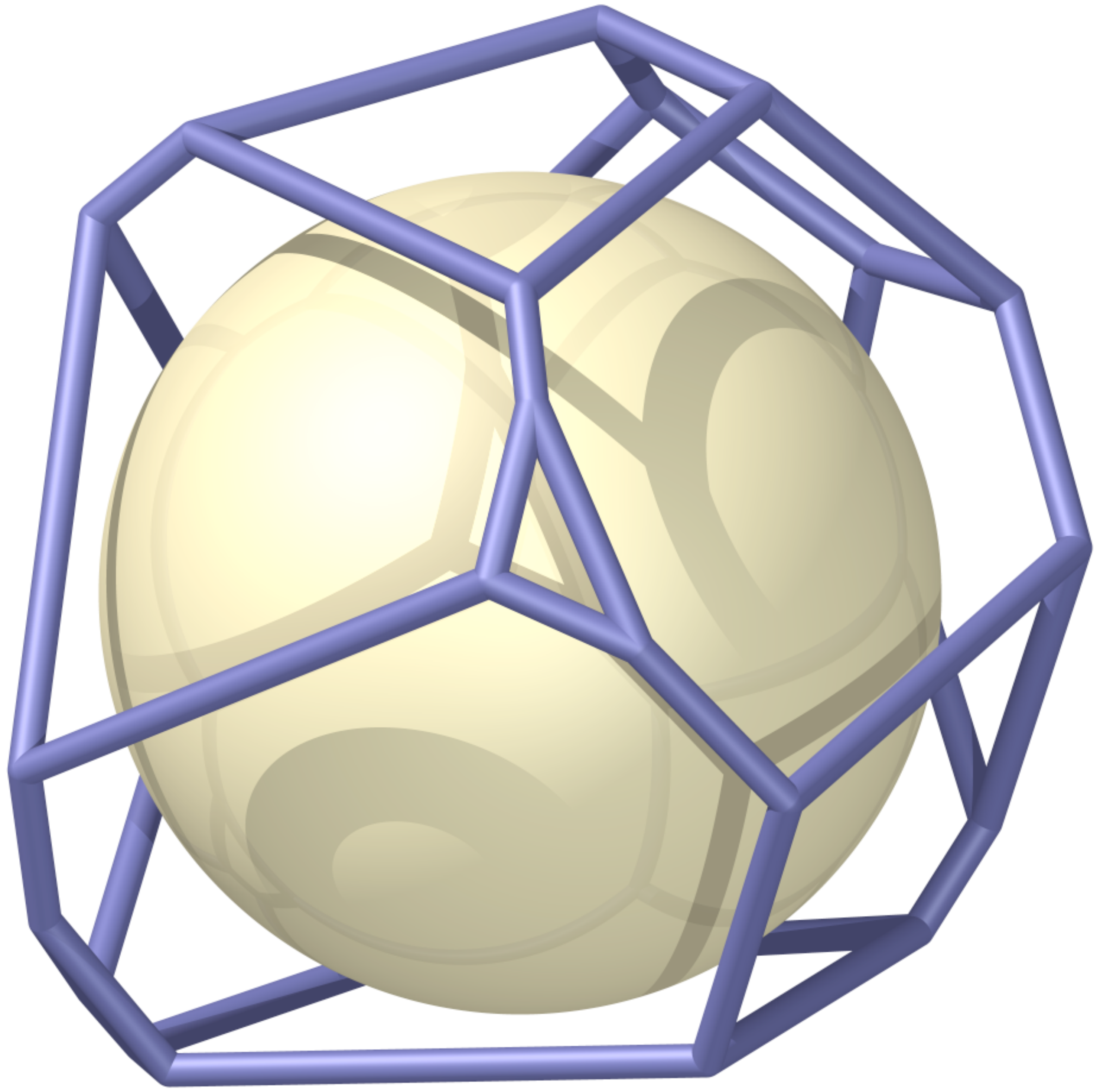
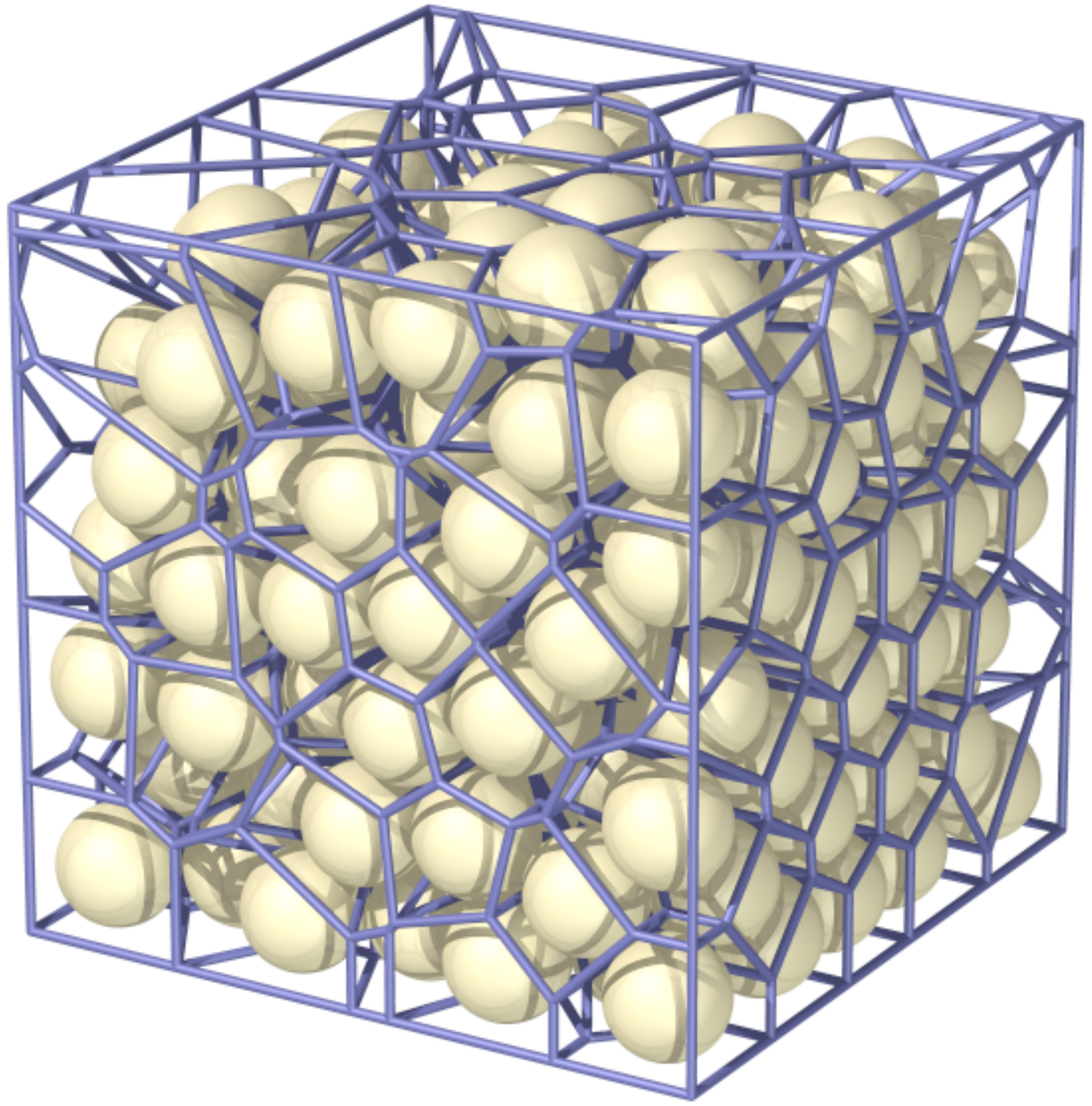
Voro++, a software library for cell-based Voronoi calculations

- Primary audience: diagnostics for particle-based simulation
- Good performance (90,000 cells per second on a typical desktop, 3x faster than Qhull)
- Written in C++ around several *classes*



voronoicell_3d class

(Code module for doing single-cell computations)

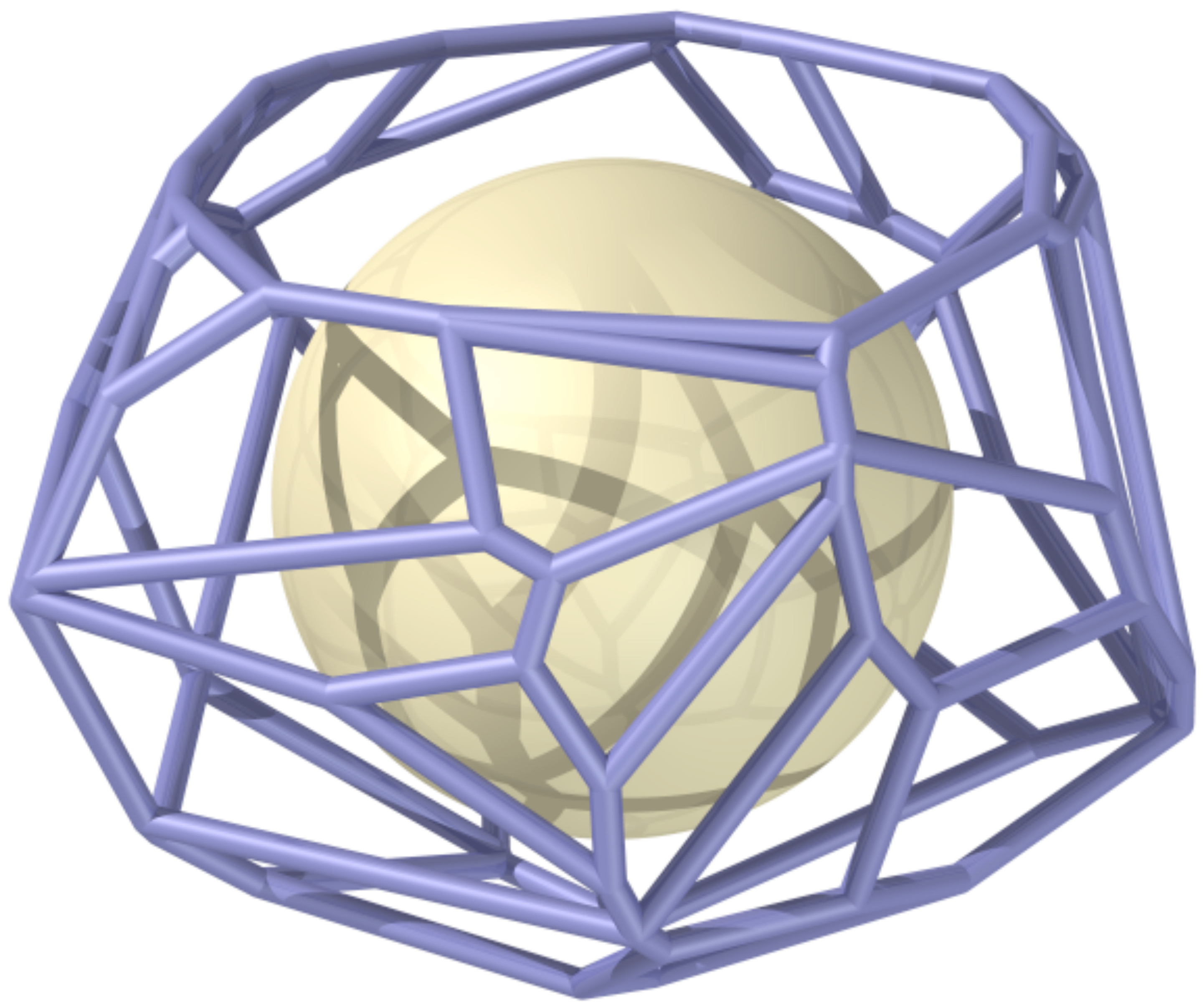


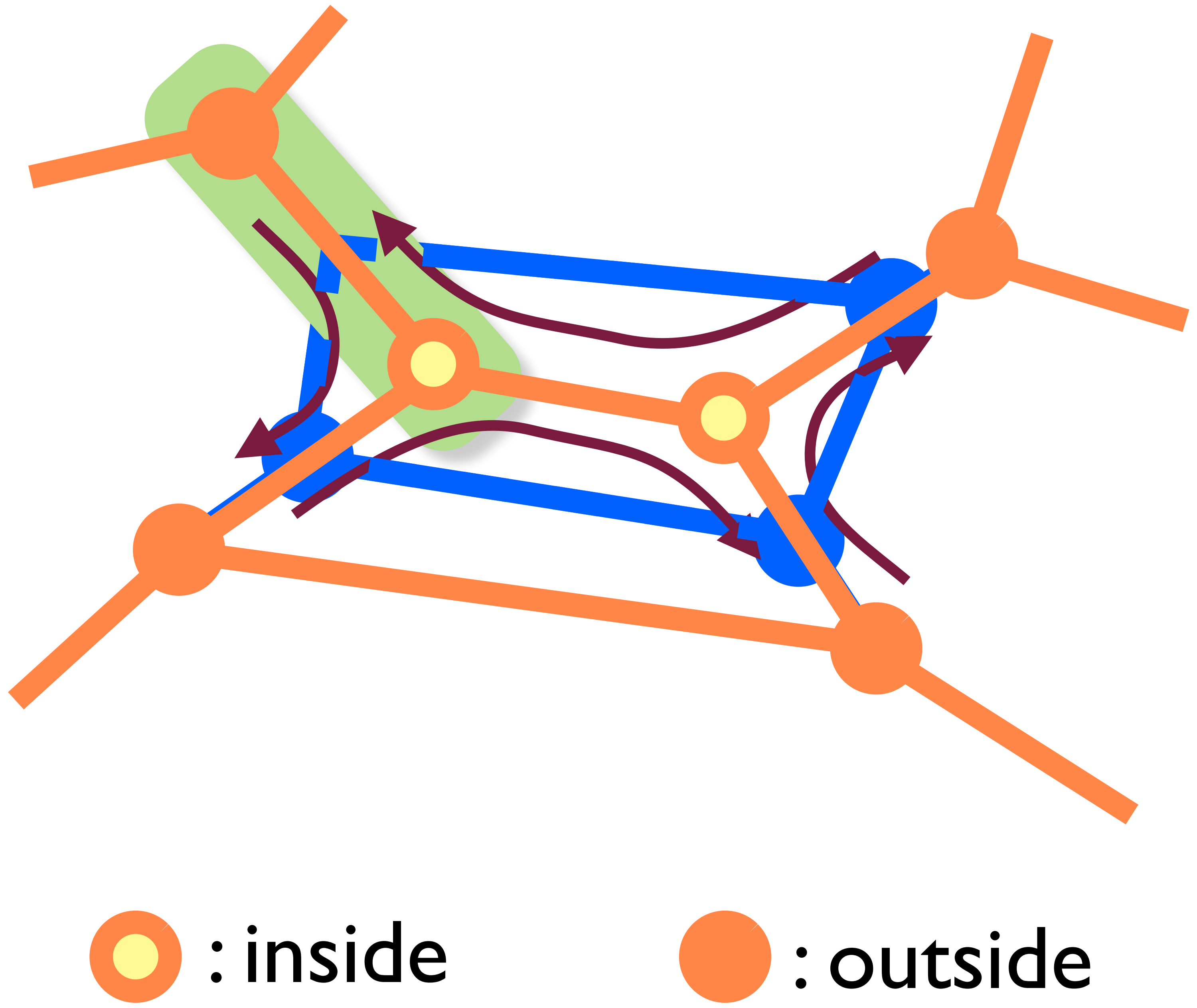
container_3d class

(Code module for Voronoi analysis of particle arrangements in a domain)

The voronoicell_3d class

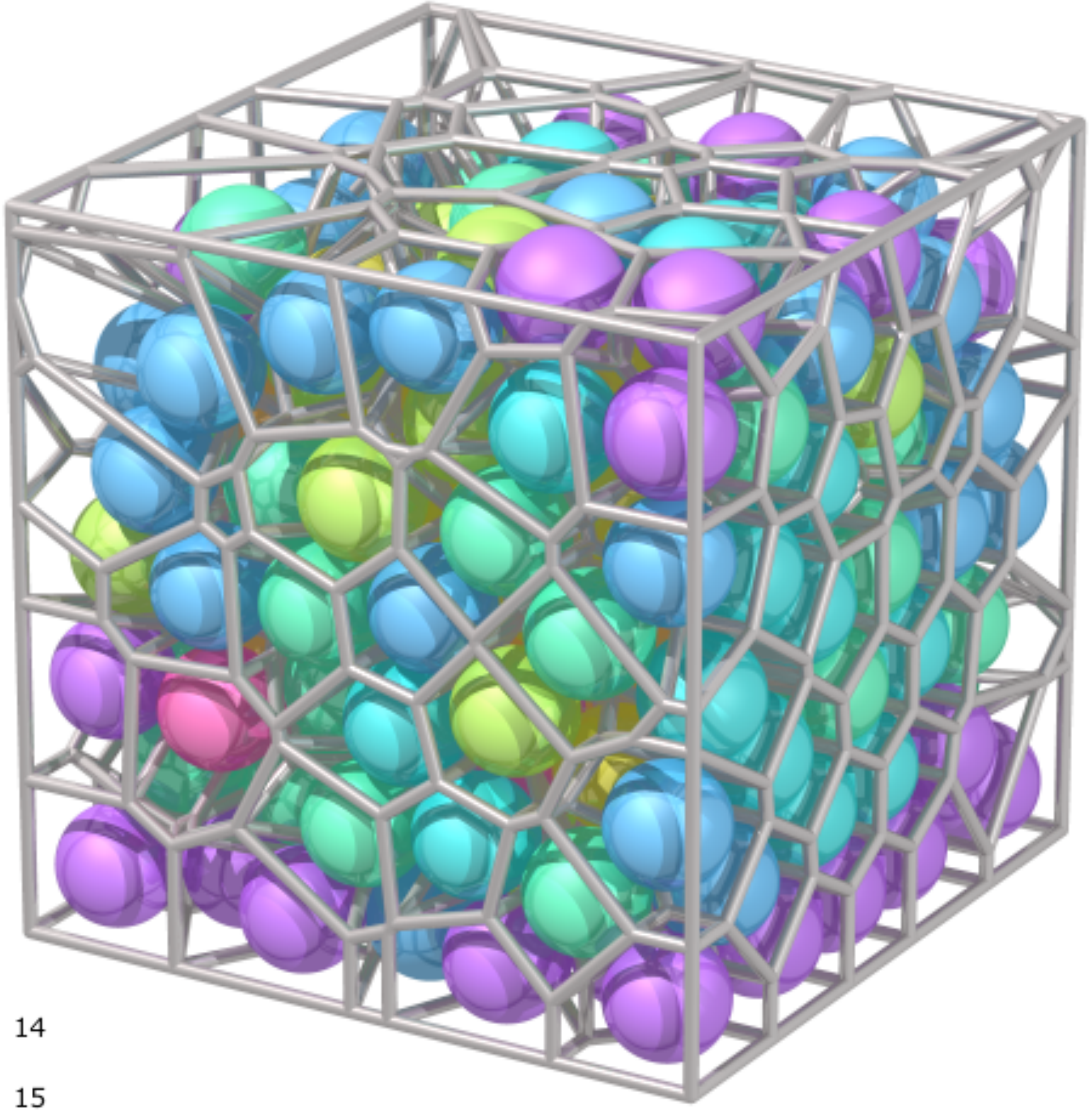
- An irregular convex polyhedron described by:
  - Vertex positions
  - Table of edges
- Primary operation: recompute vertices when cut by a plane
- Diagnostic routines:
  - Number of planes, edges
  - Volume, centroid, *etc.*





The container_3d class

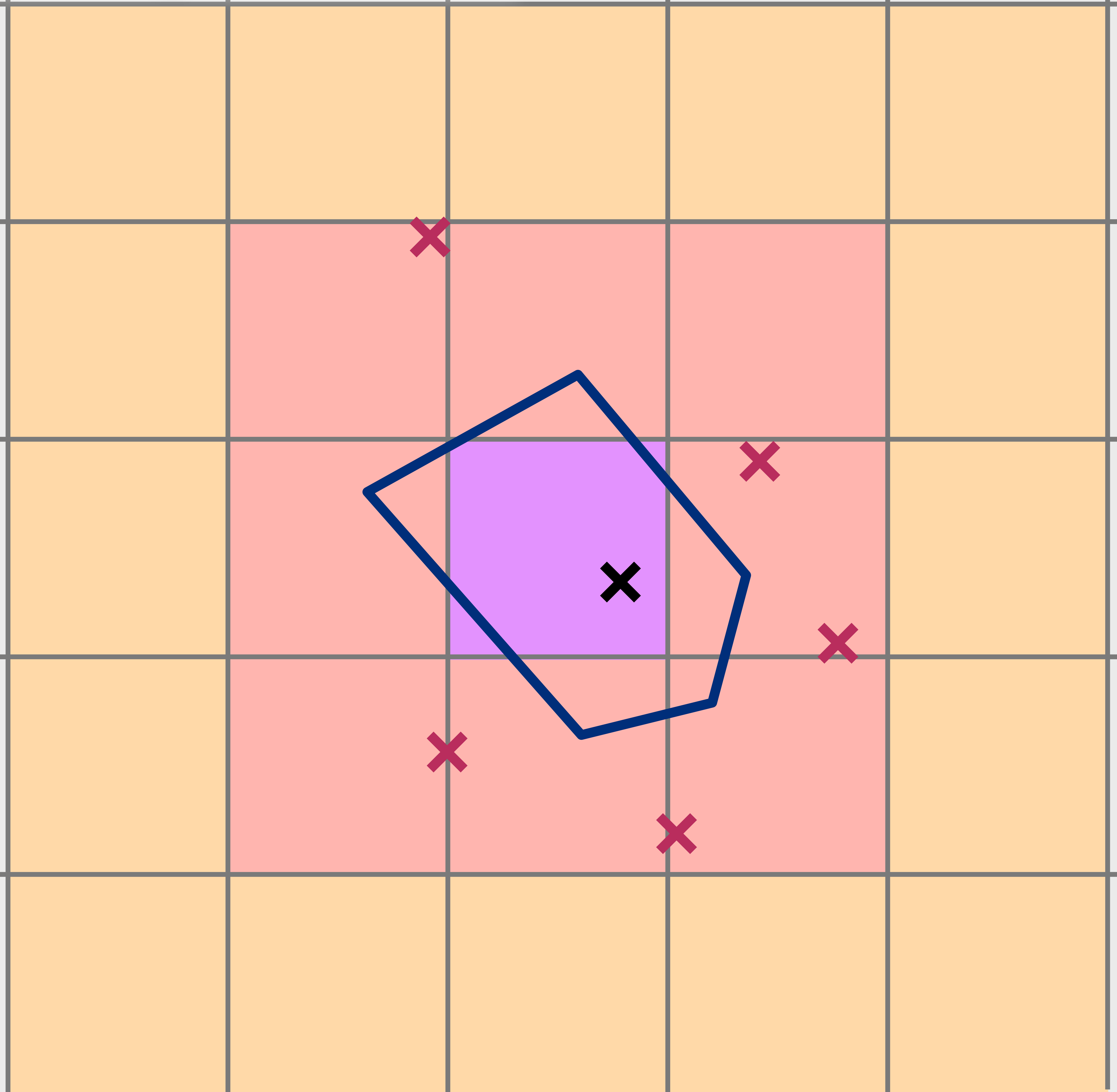
- Sorts particles into rectangular grid of blocks
- Uses voronoicell class to construct individual cells by testing over the blocks
- Can carry out a variety of calculations on the computed cells
- Library and example programs available for download from http://math.lbl.gov/voro++/



Voronoi tessellation with 216 particles in a cube of side length 6, generated by DEM simulation

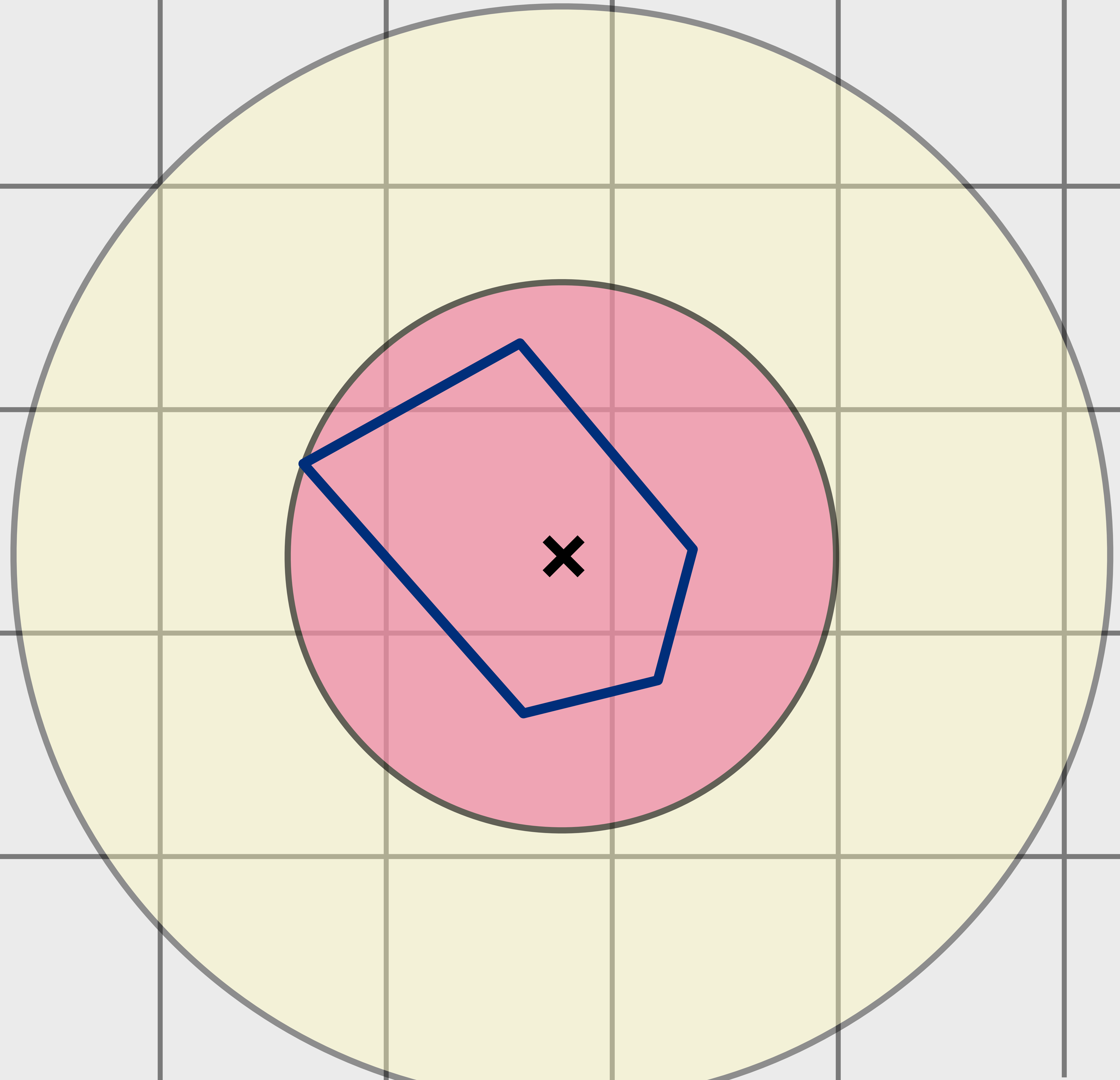
Internal 3 x 3 x 3 grid of particles colored according to computation blocks the Voronoi cell faces

A hybrid searching algorithm



Basic approach: sweep outwards and apply plane cuts for particles in those blocks

A hybrid searching algorithm



Sphere bounding: only need to test blocks up to twice the maximum distance to a vertex

A hybrid searching algorithm

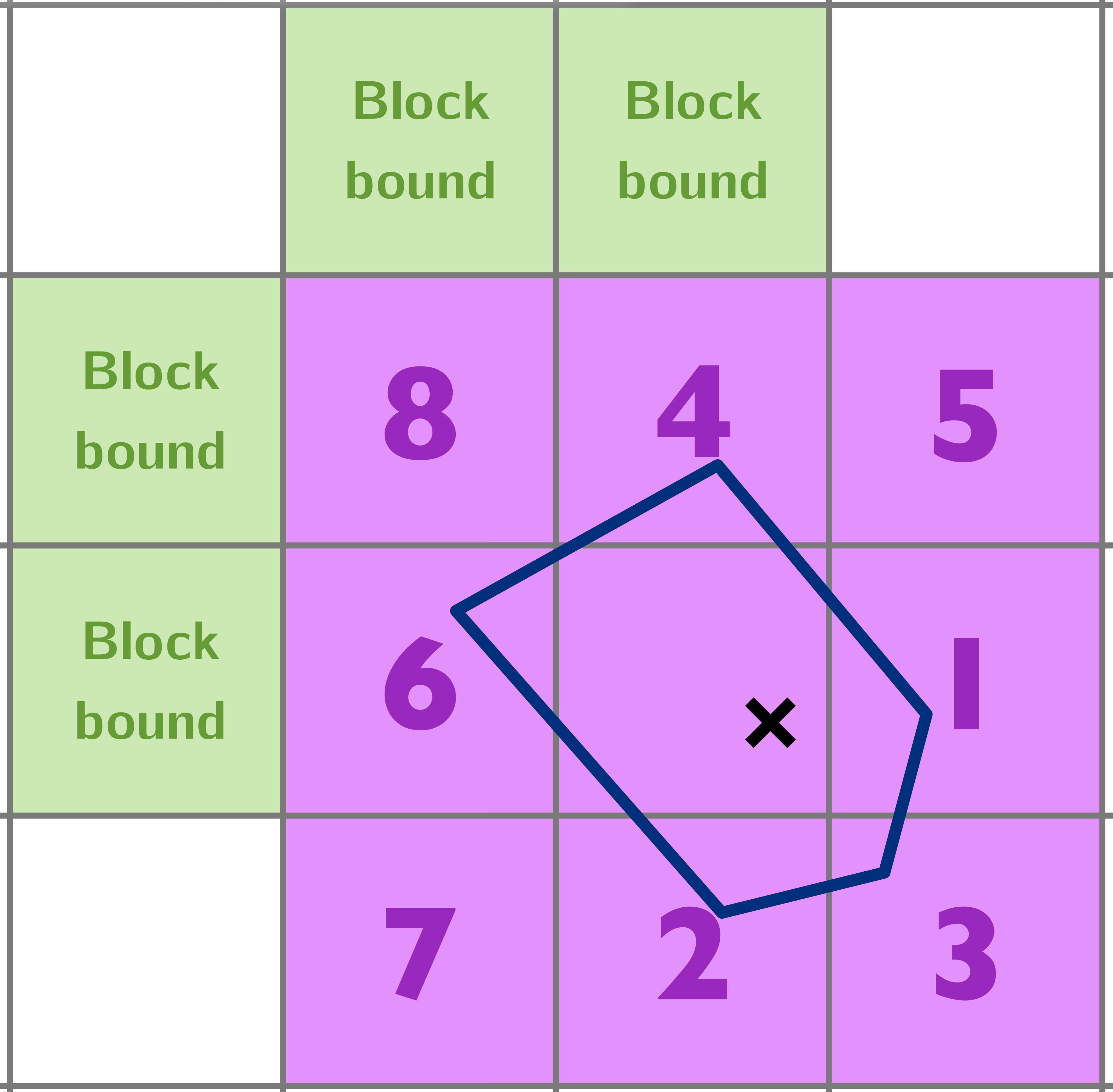
Advantage: very fast

Disadvantage: works poorly for cells that extend far in one direction

A hybrid searching algorithm

Block bounding: apply plane tests to ascertain if a block could possibly cut the cell

A hybrid searching algorithm

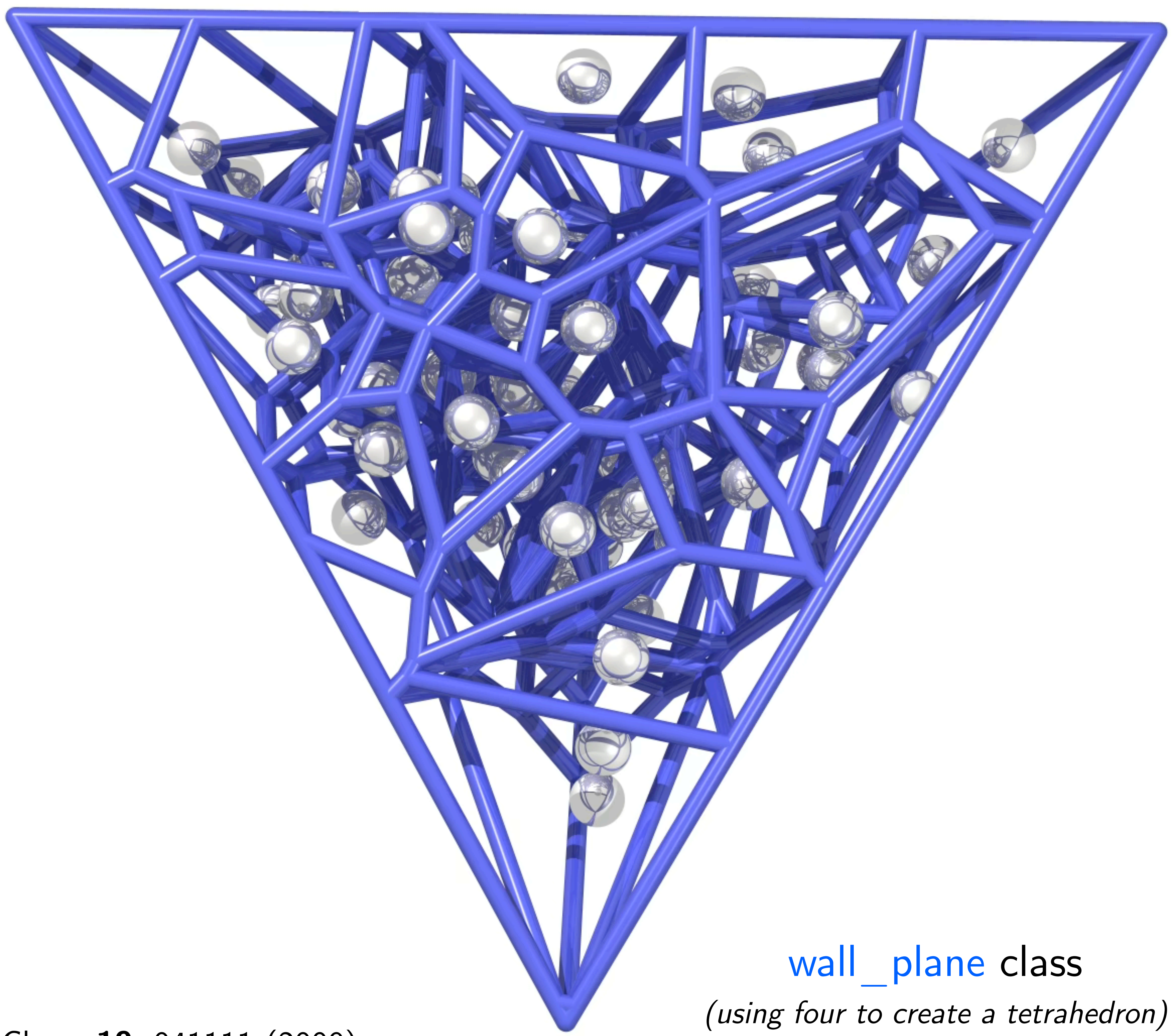


Hybrid approach:

1. Apply a precomputed list of nearby blocks, using sphere bounding
2. Flood fill outwards using block bounding

Classes for wall computations

- Wall classes can be added to the container class
- They apply additional plane cuts during cell construction
- Gives perfect results within convex polygonal shapes



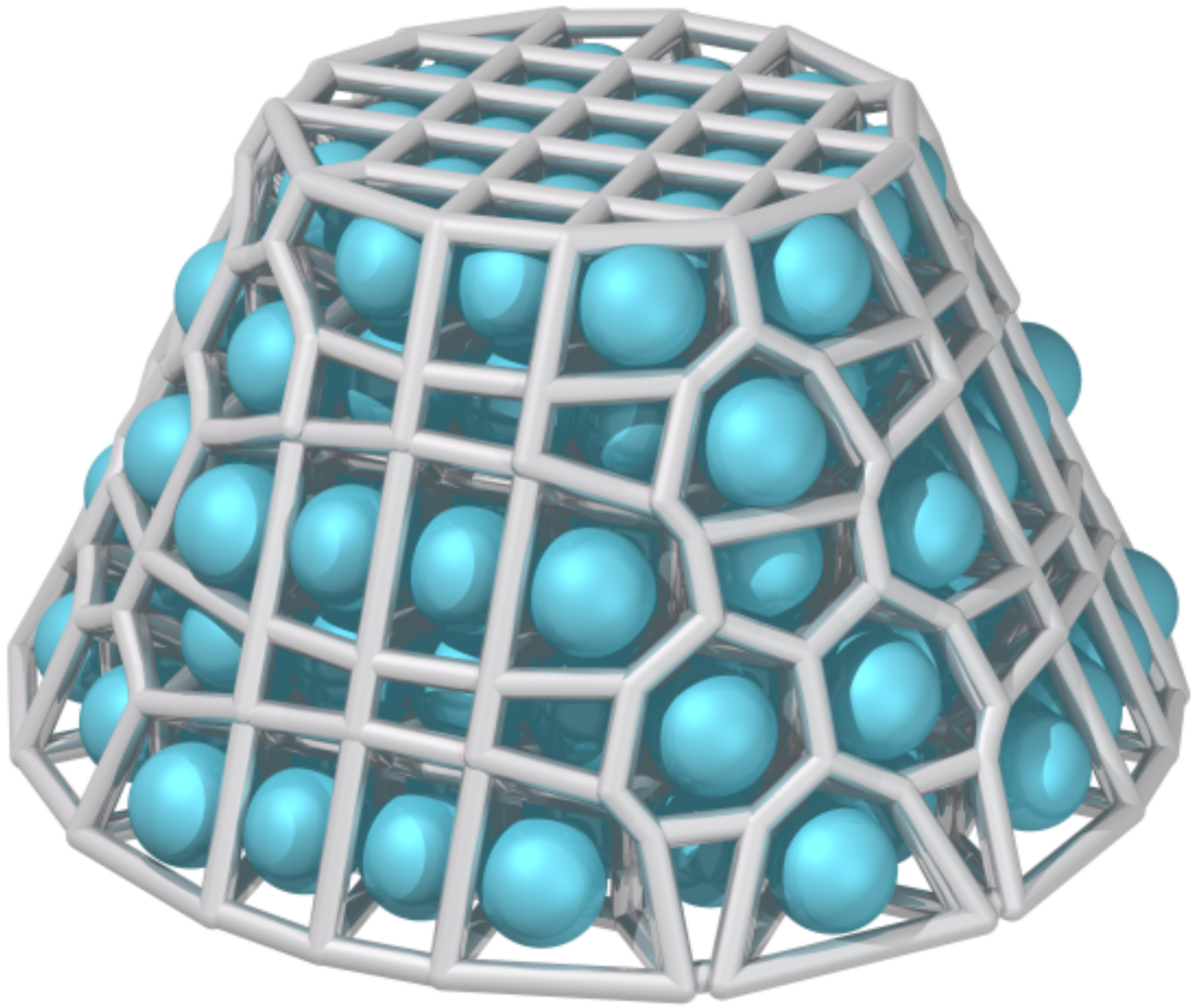
wall_plane class

(using four to create a tetrahedron)

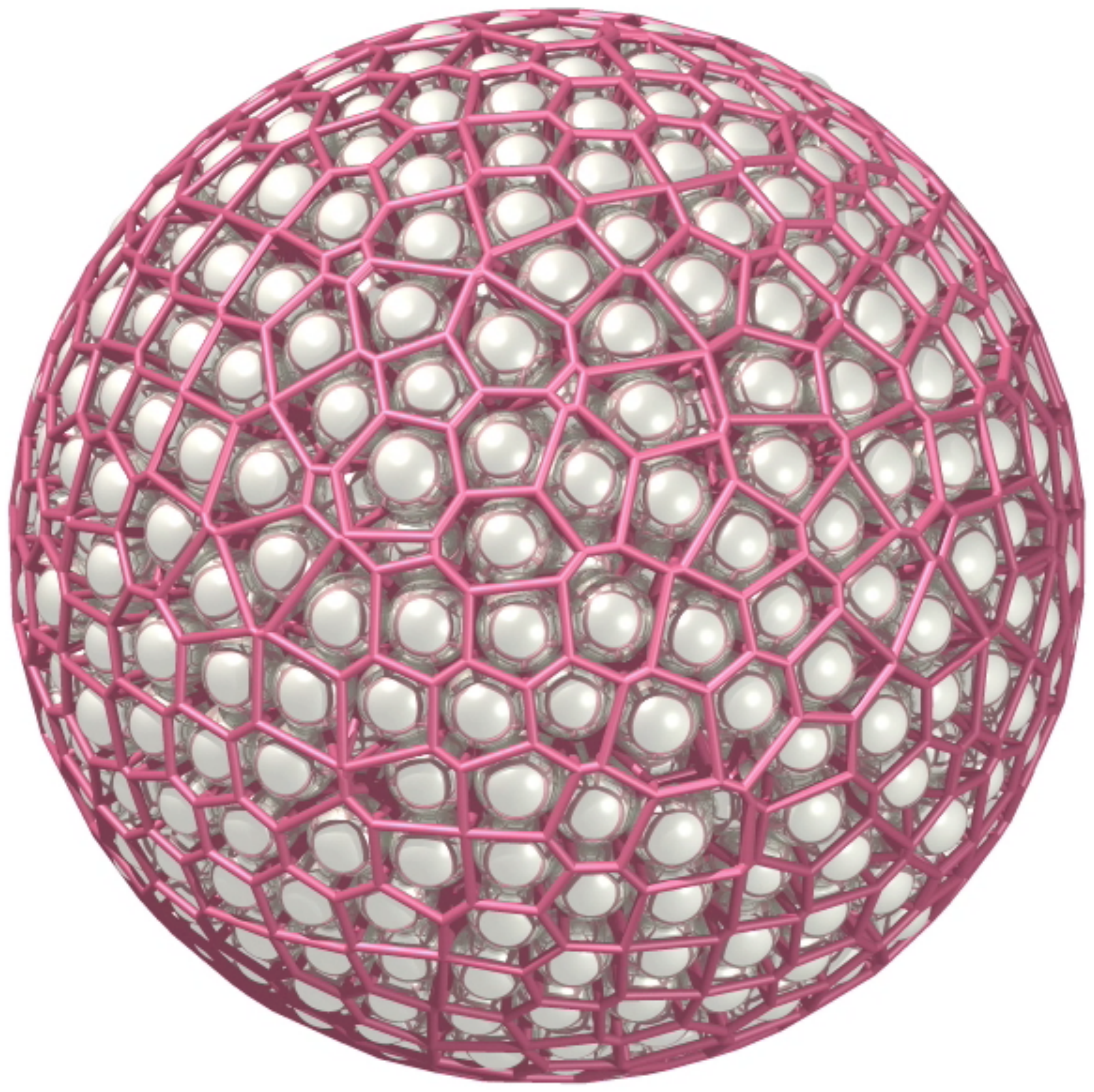
C. H. Rycroft, *Voro++: A three-dimensional Voronoi cell library in C++*, Chaos **19**, 041111 (2009).

Walls with curved boundaries

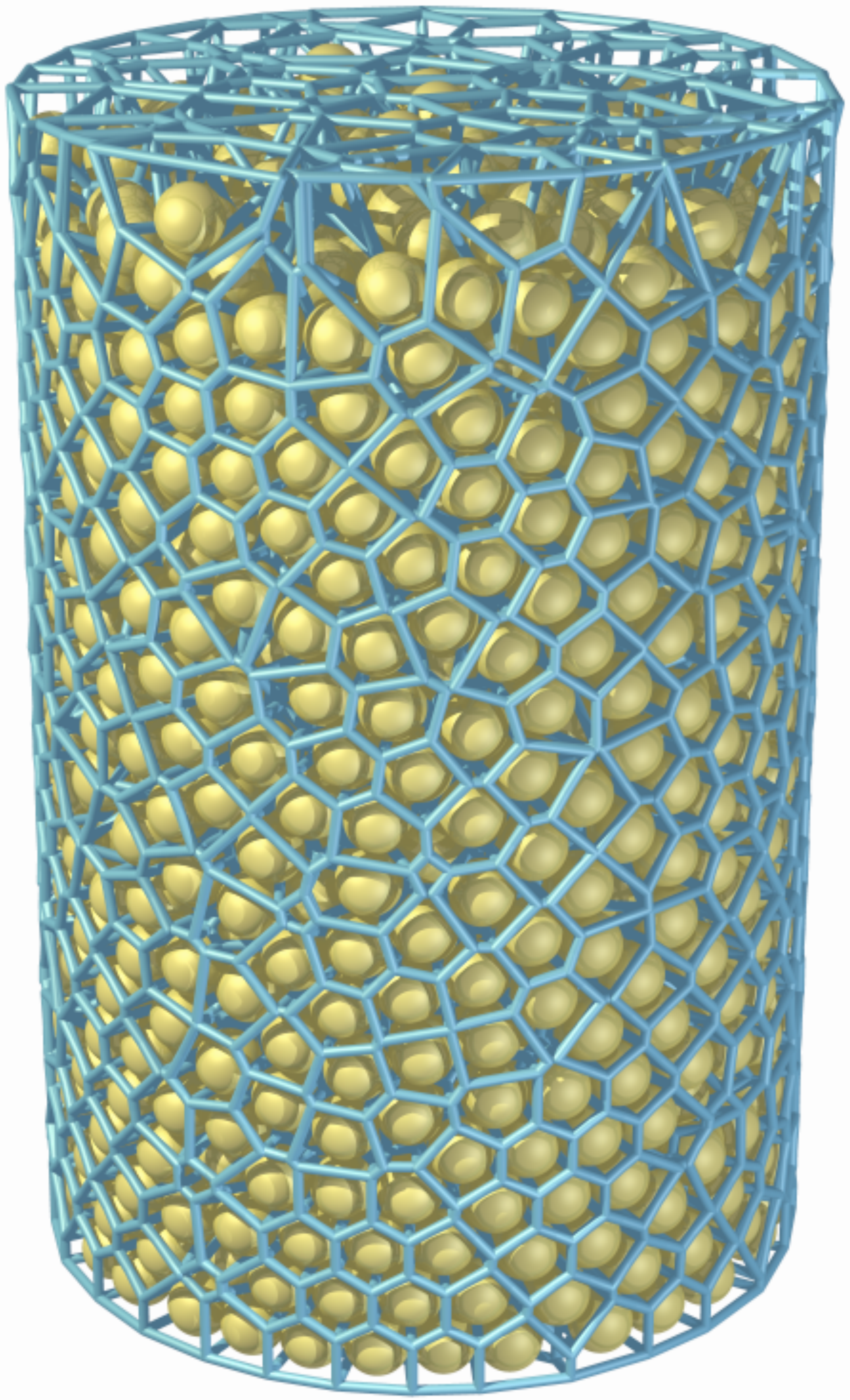
- Curved boundaries can be approximated with plane cuts
- Has small inaccuracies from approximating the curved surface



wall_cone class
(to make a frustum)



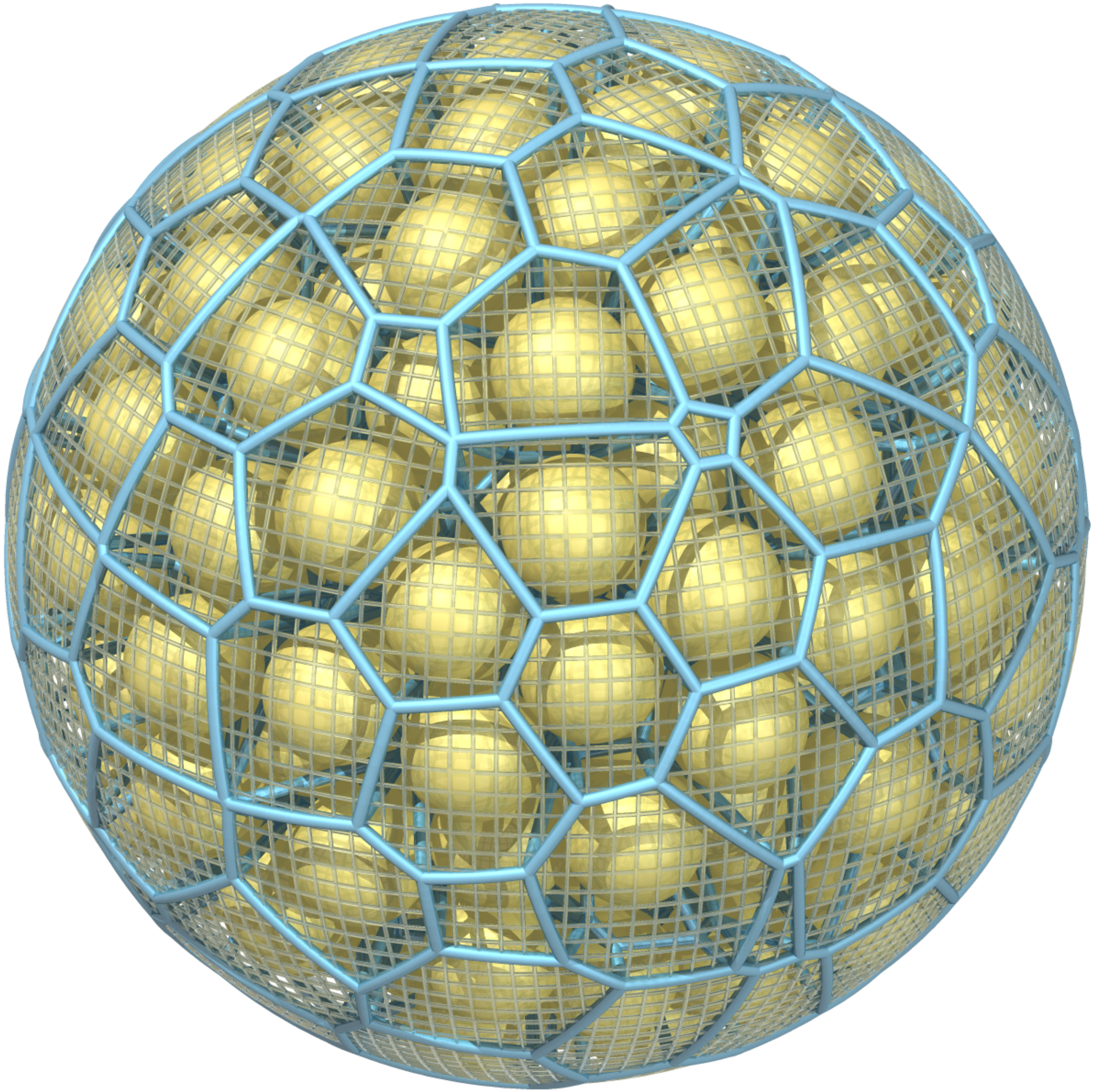
wall_sphere class



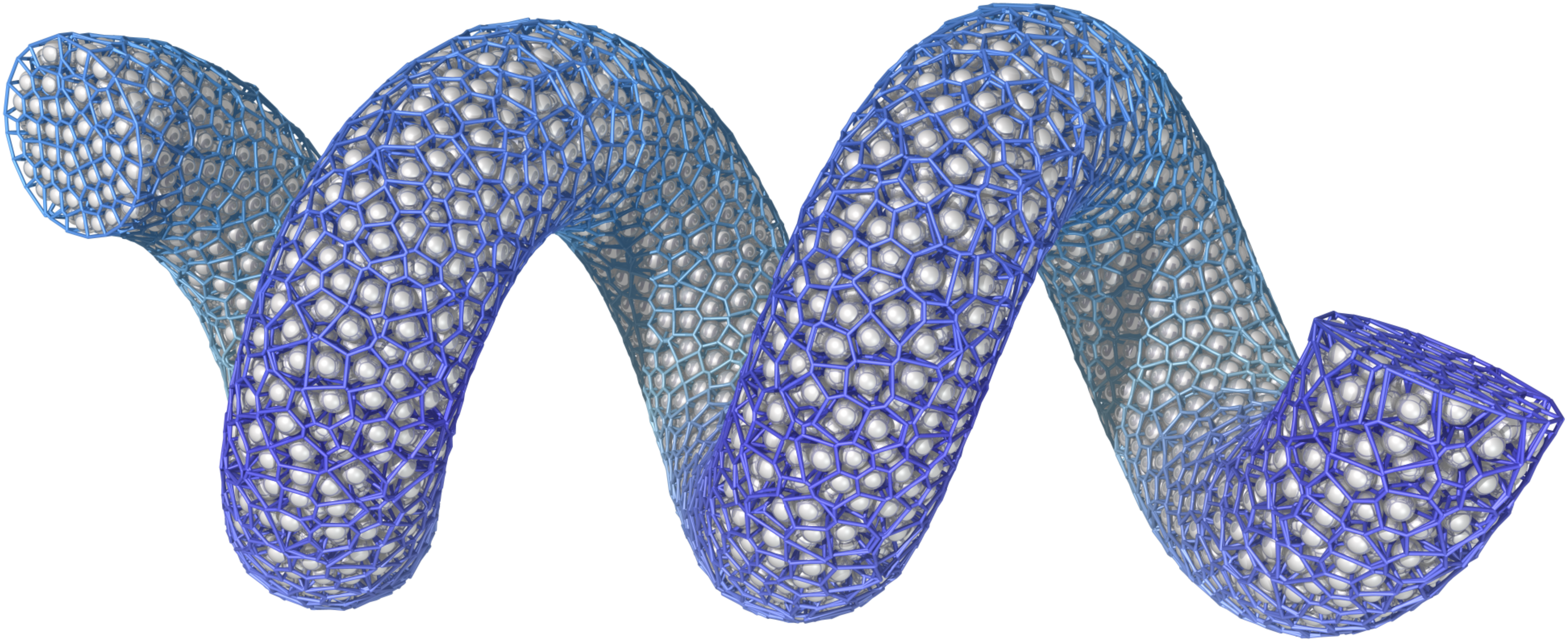
wall_cylinder class

Higher accuracy

- Multiple plane cuts can better approximate a curved surface
- In the example shown, a 2D grid of cutting planes is applied to every Voronoi cell
- The total Voronoi cell volume differs from the exact sphere volume by 0.039%

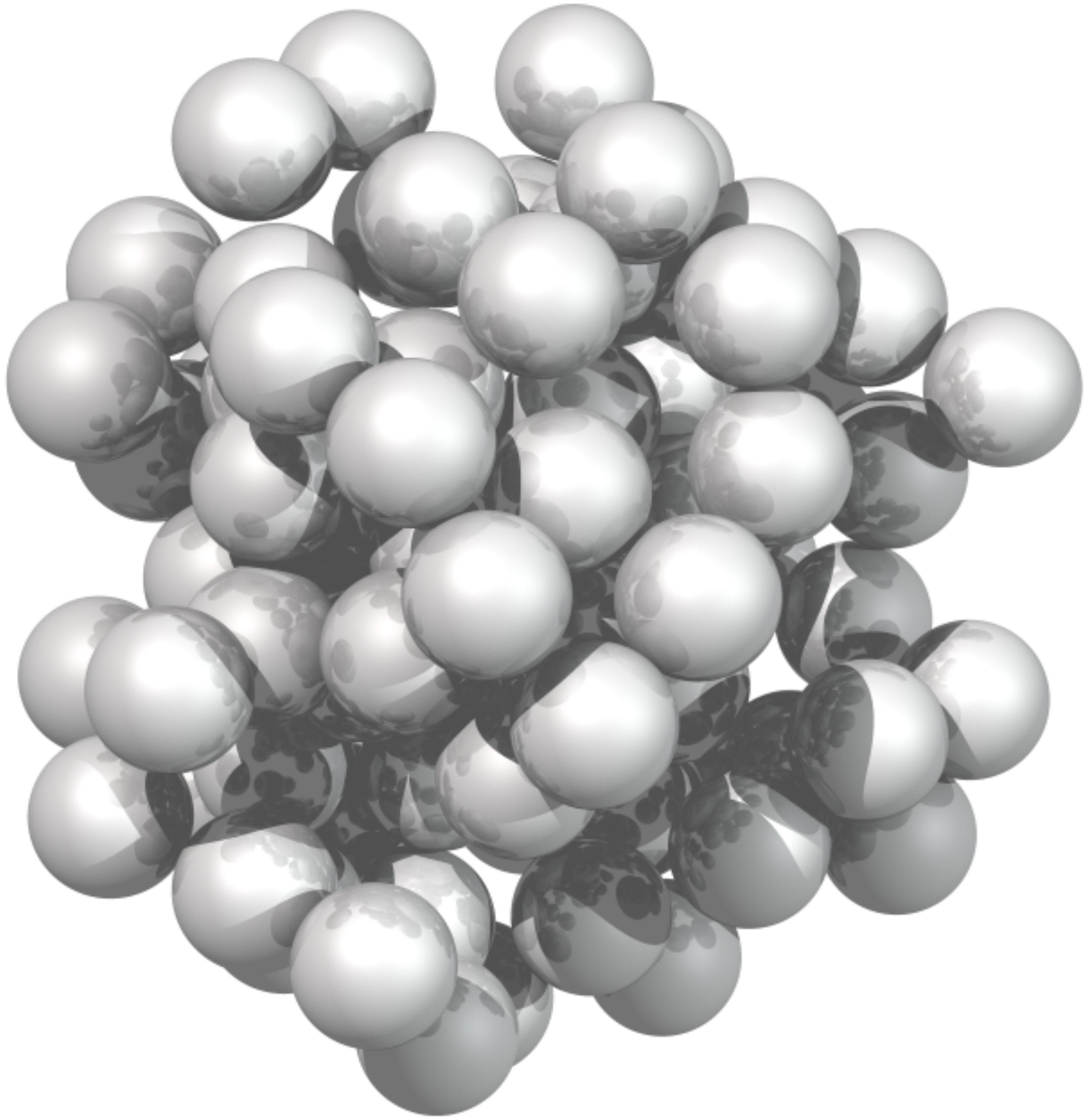


Custom wall shapes



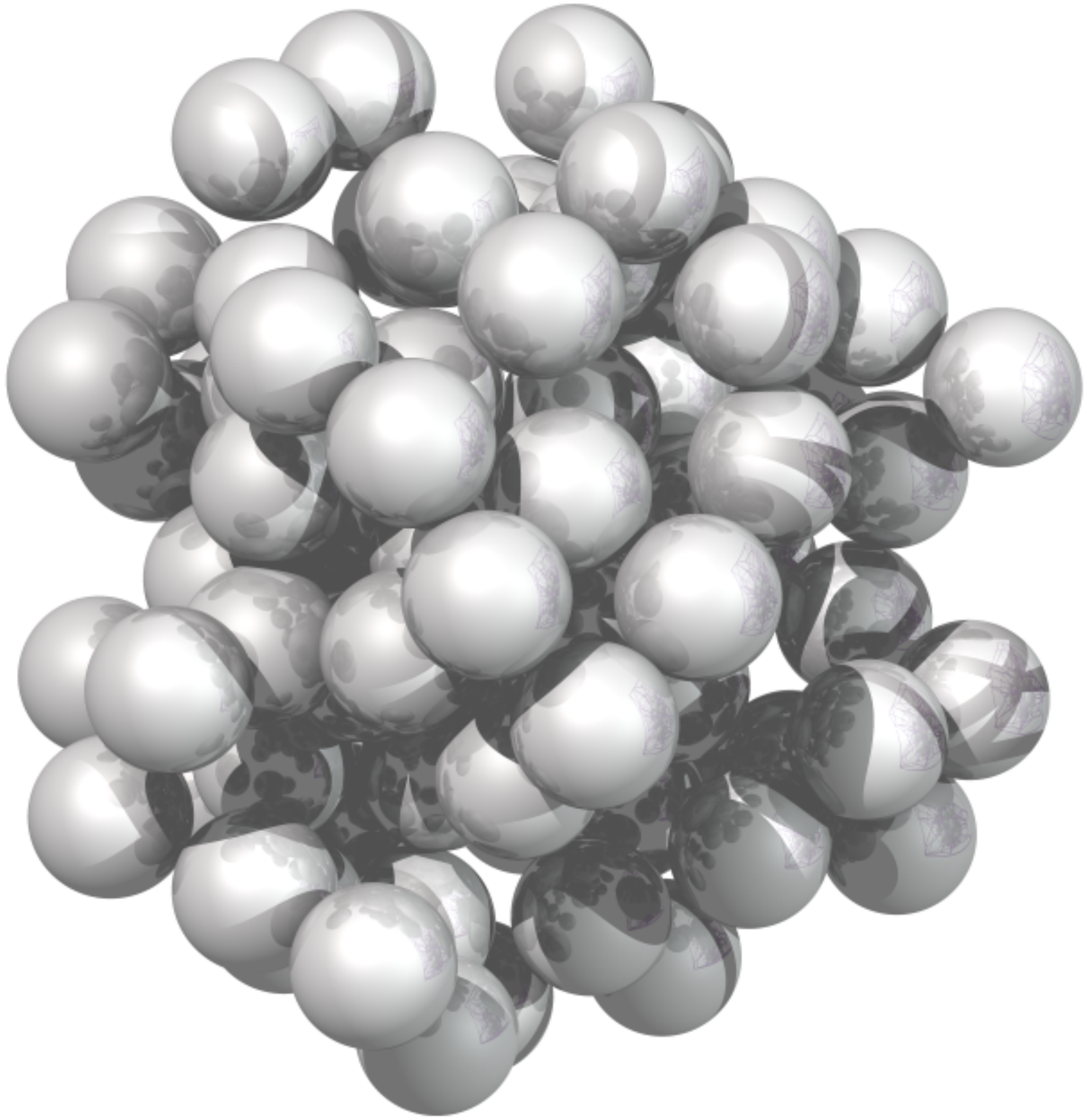
Additional wall shapes can be written by the user to handle custom domains

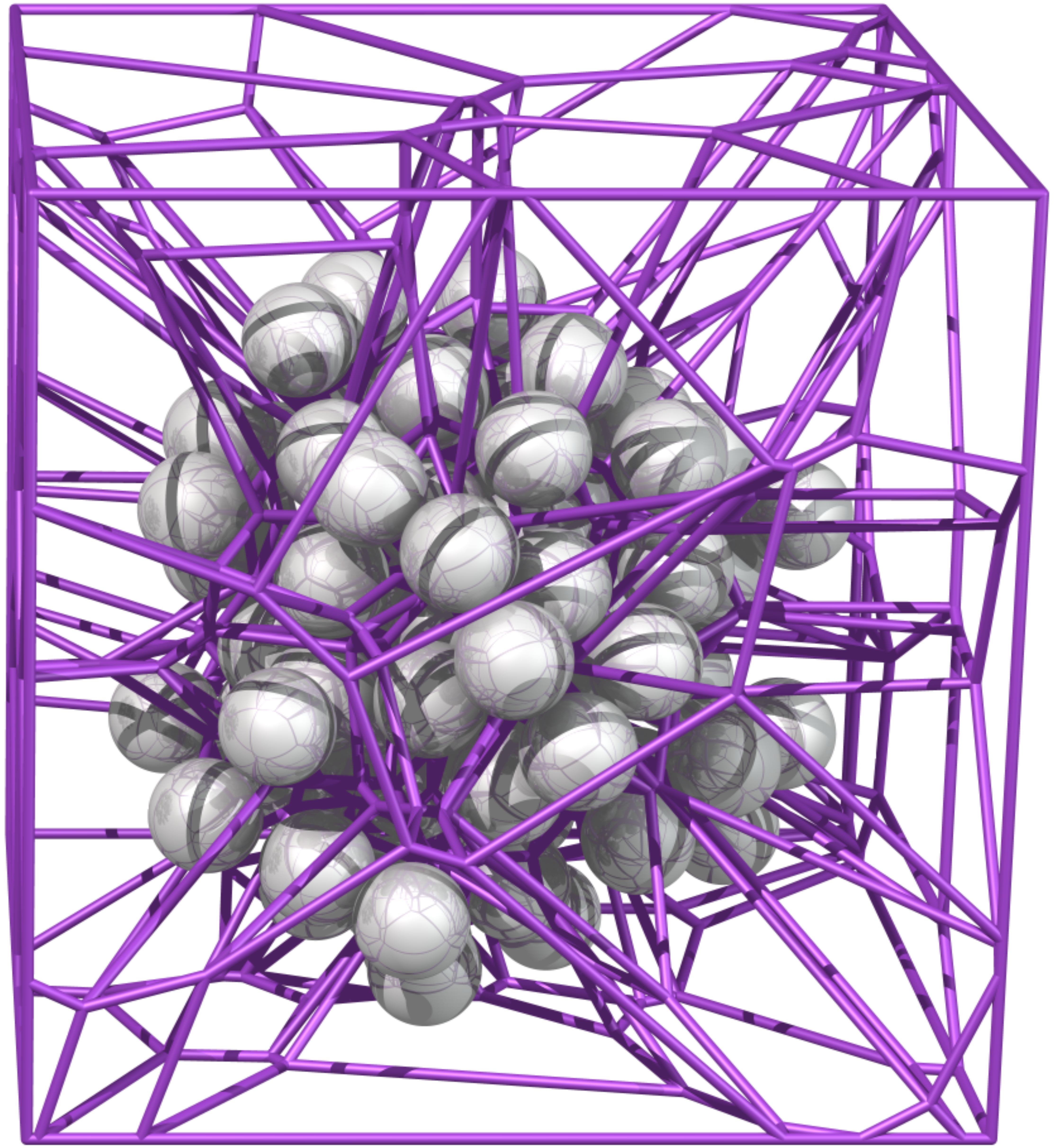
Irregular particle packings



- Another common scenario is to have particles that form an irregular arrangement in space
- These may not conform to any particular domain
- Voronoi cells may extend much further than the arrangement itself

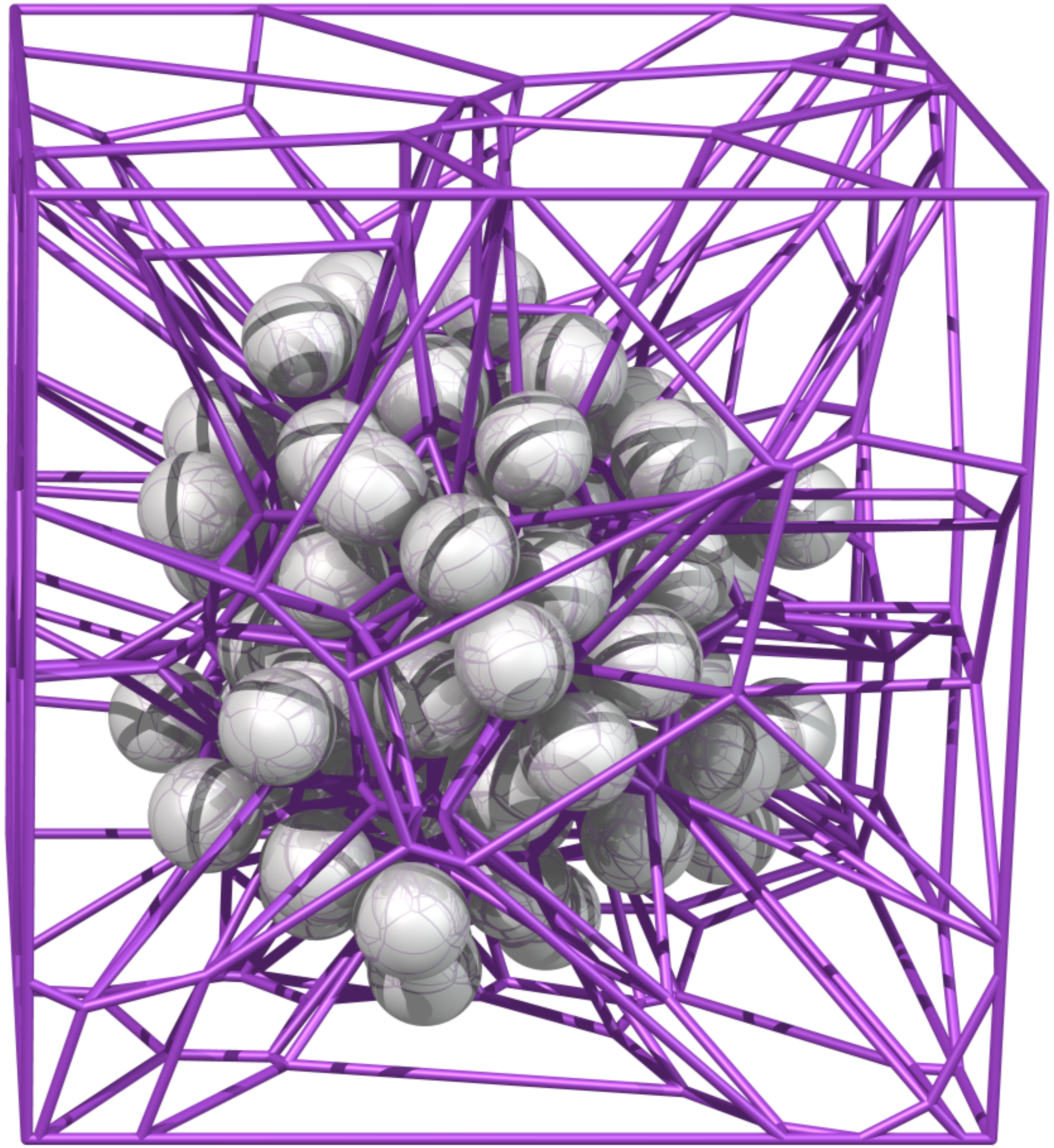
Irregular particle packings





Irregular particle packings

- May have negative consequences for analysis:
  - Very large Voronoi cell volumes for particles on the periphery
  - Large numbers of Voronoi faces, which may difficult to interpret physically
  - Neighbor connections between particles that are far away



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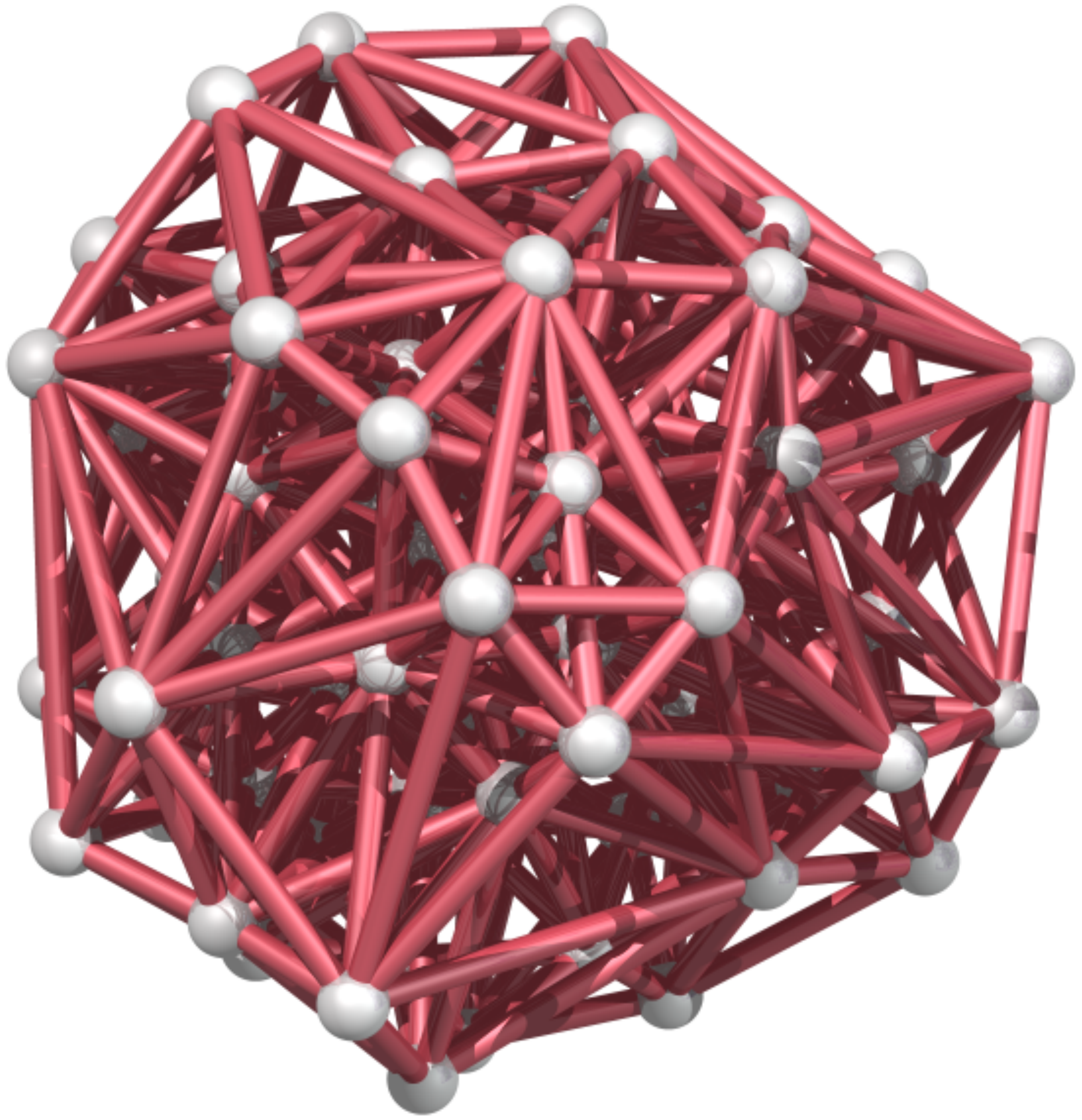
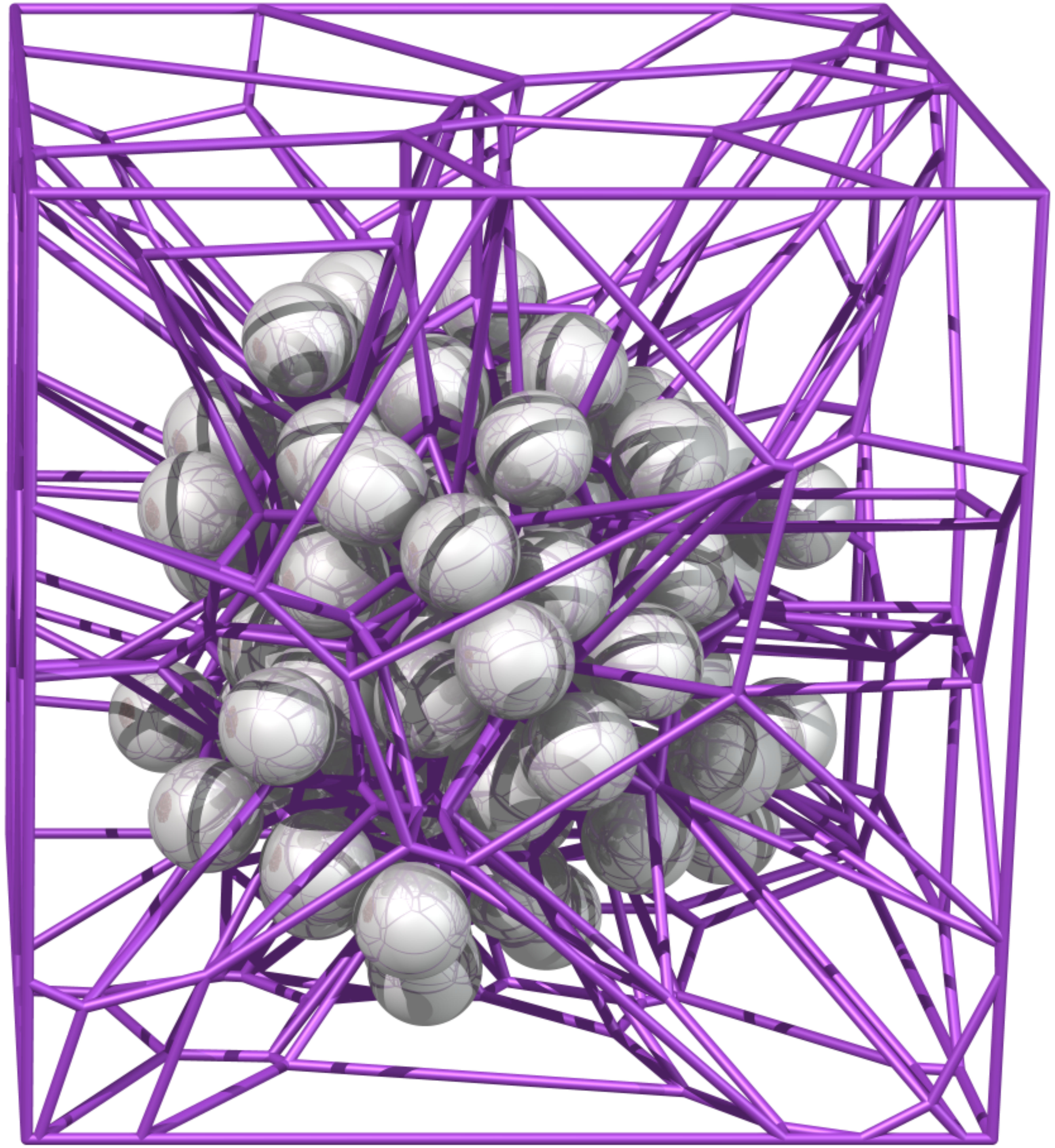


Neighbor relations are shown in red

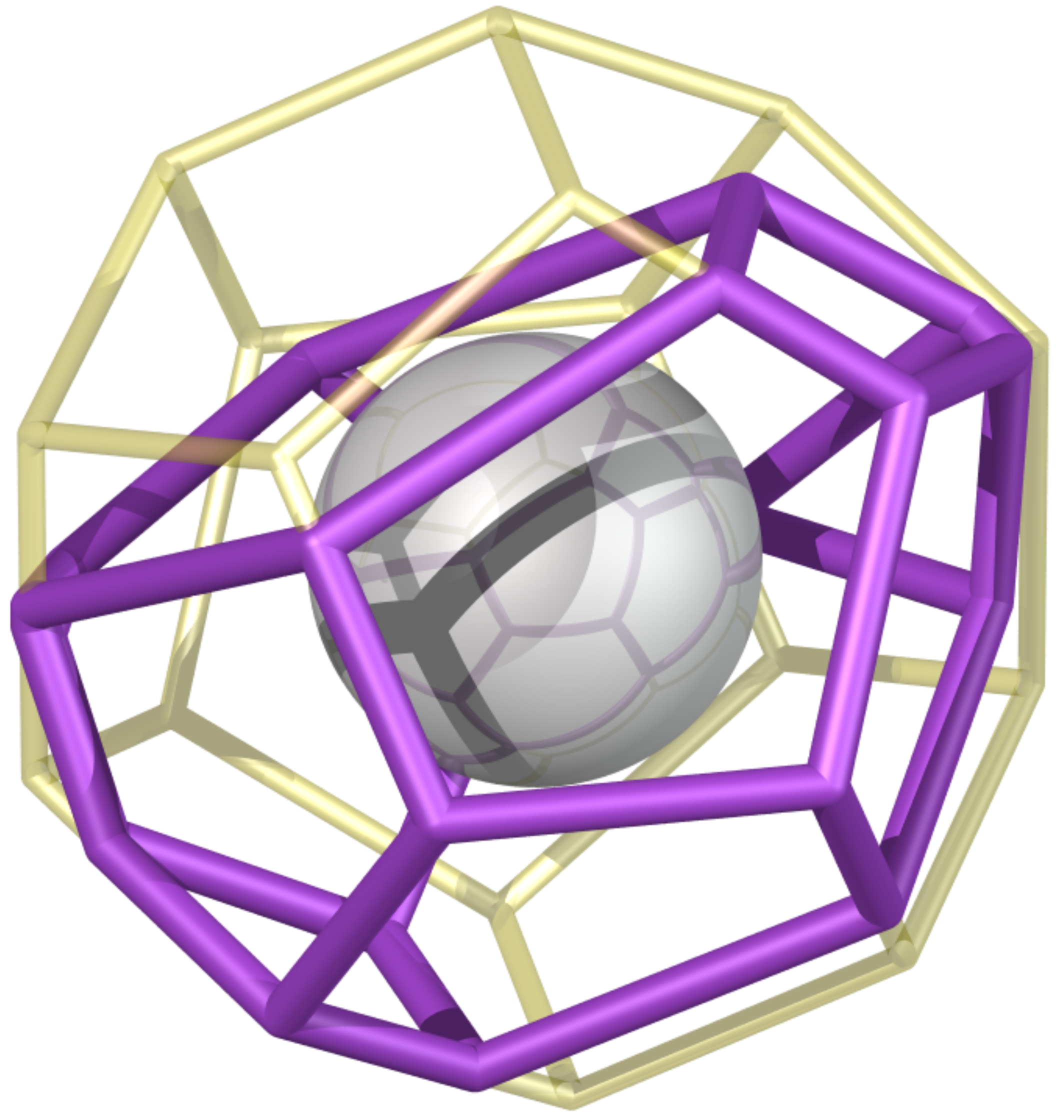


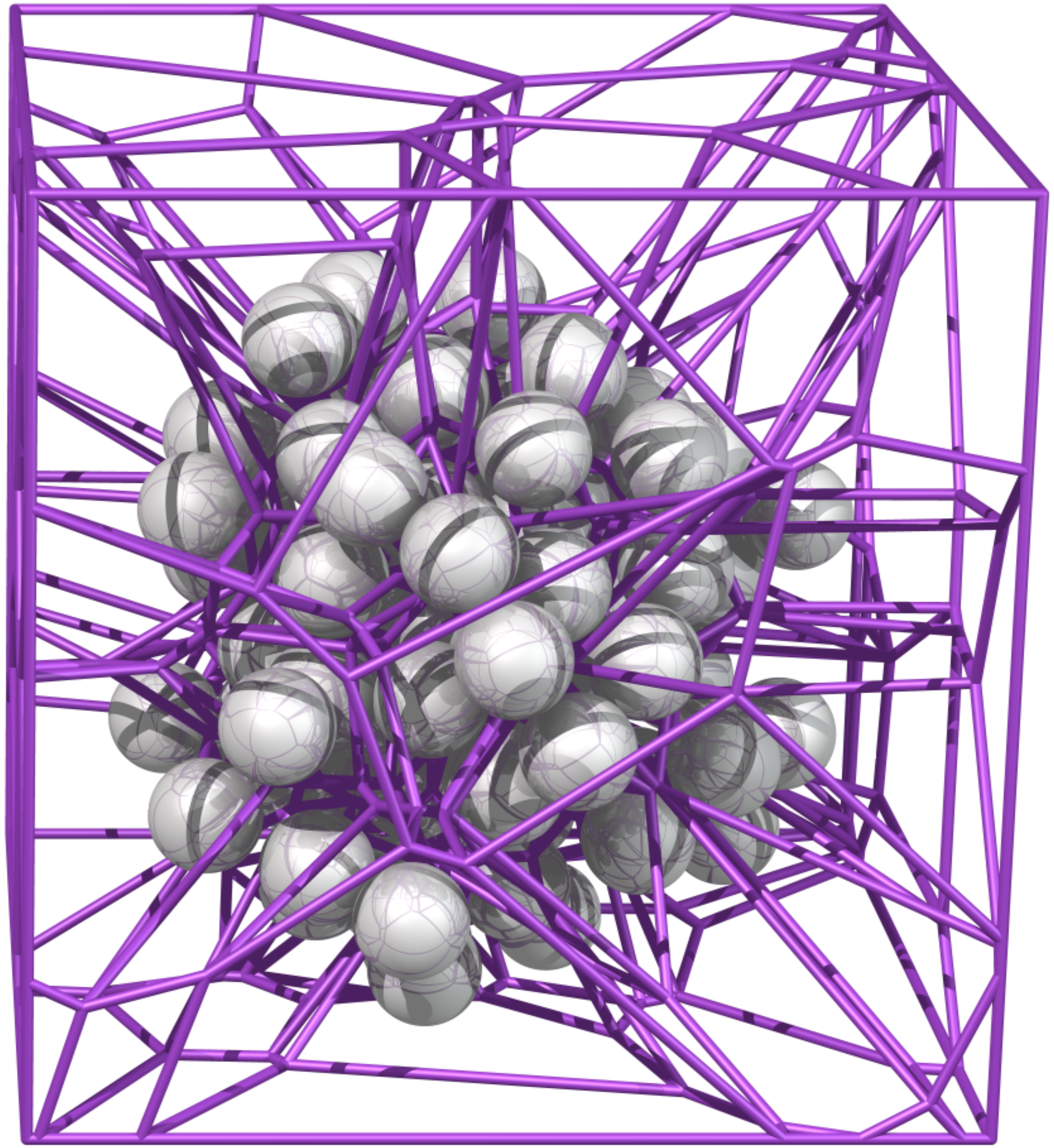
Irregular particle packings

- Usually each Voronoi cell is initialized to fill the entire domain
- Alternative scenario: start each Voronoi cell as a reference shape (e.g. a dodecahadron)

Yellow lines
indicate initial shape

Purple lines
indicate Voronoi cell after plane cuts



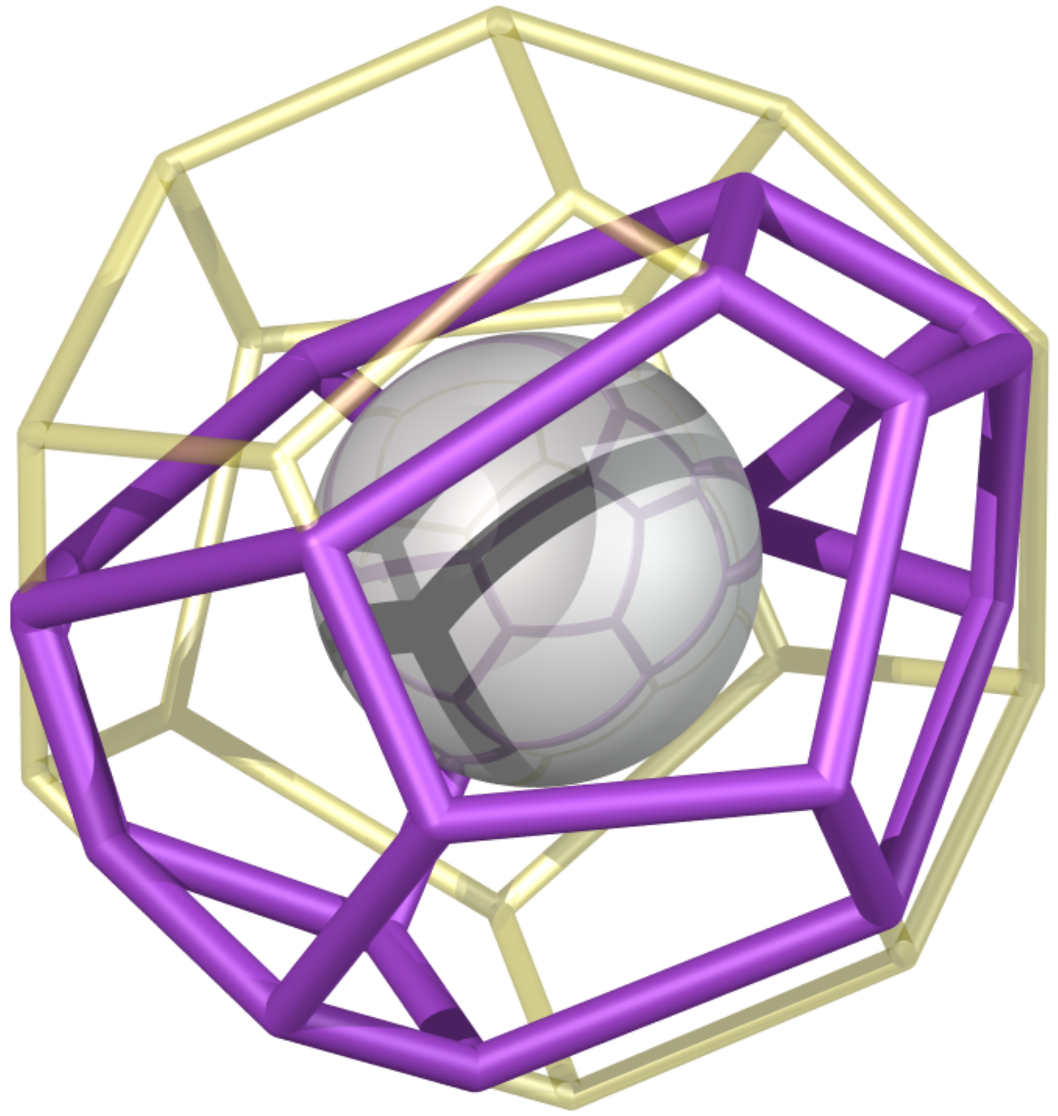


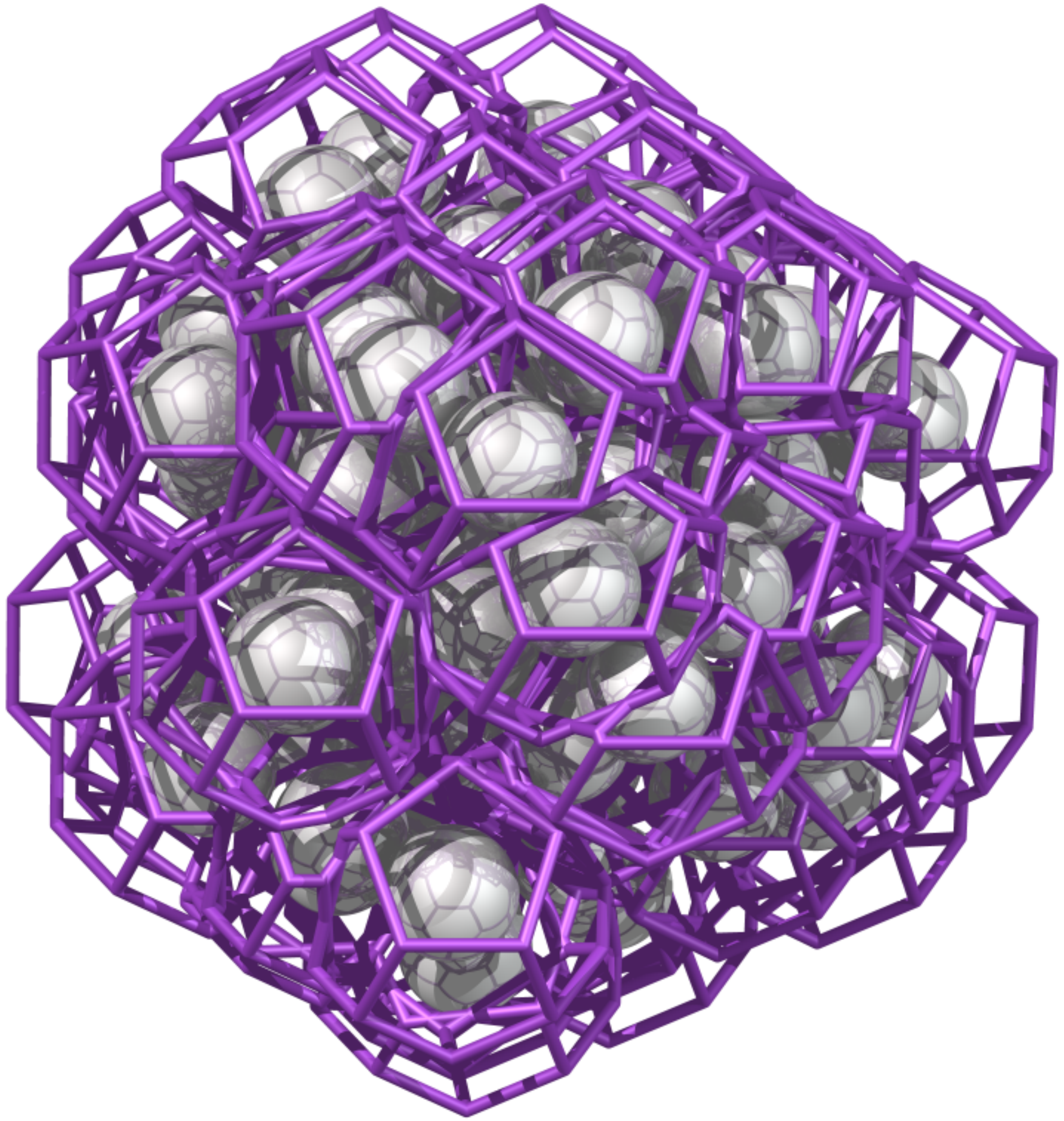
Irregular particle packings

- With this method, the Voronoi cell structure conforms to the packing arrangement
- More efficient to compute, since small cells require less searching

Yellow lines
indicate initial shape

Purple lines
indicate Voronoi cell after plane cuts





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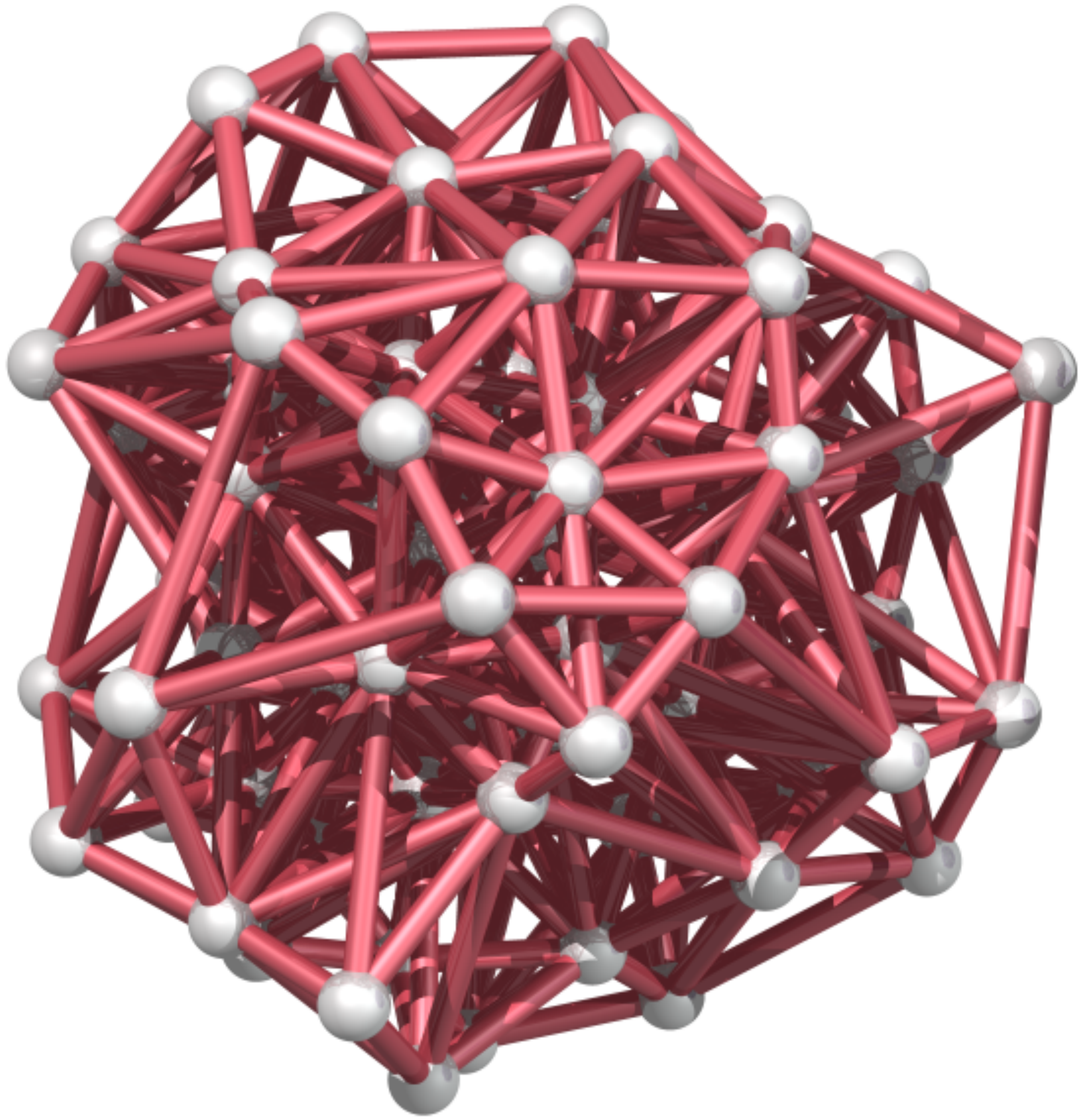

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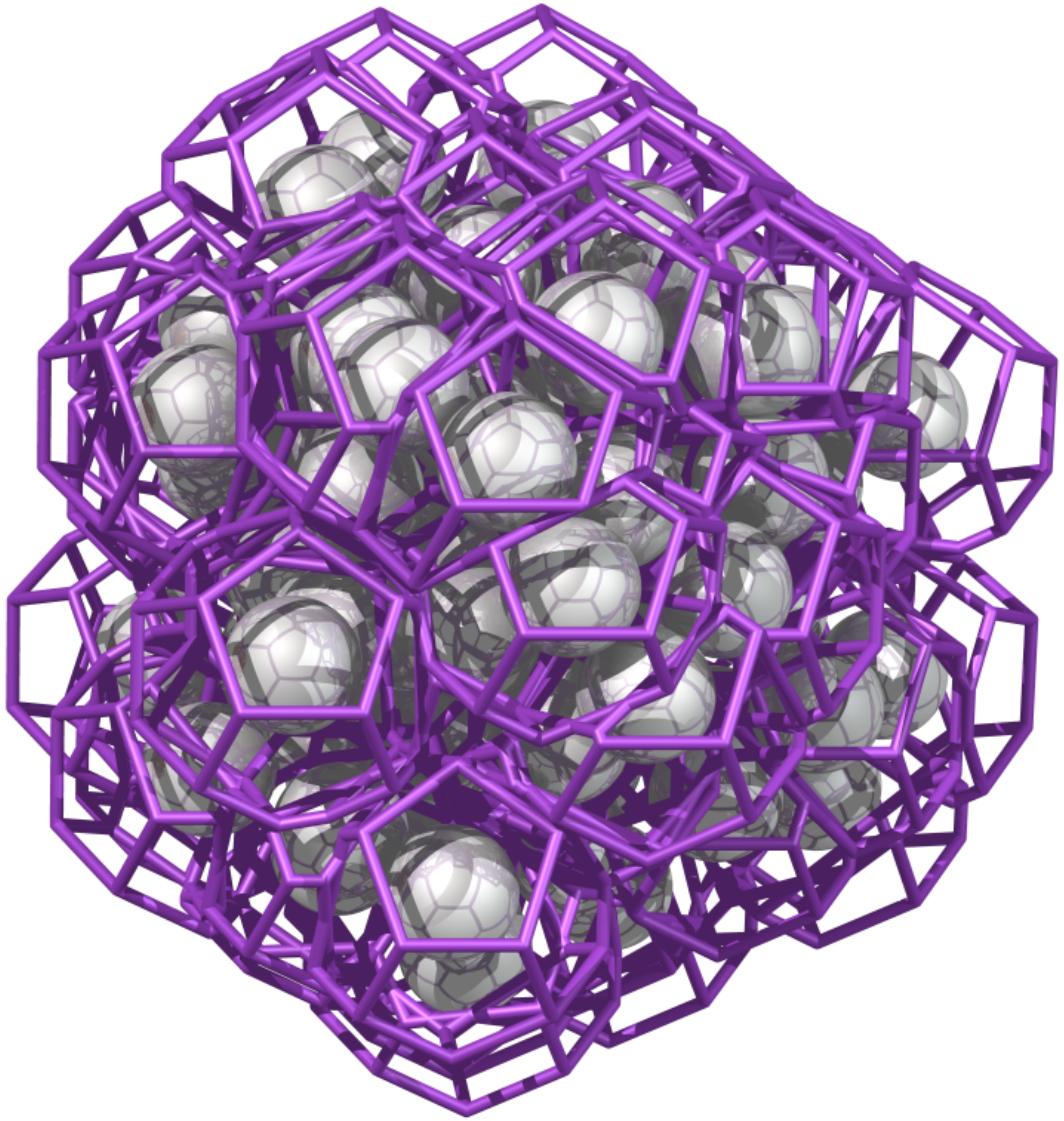

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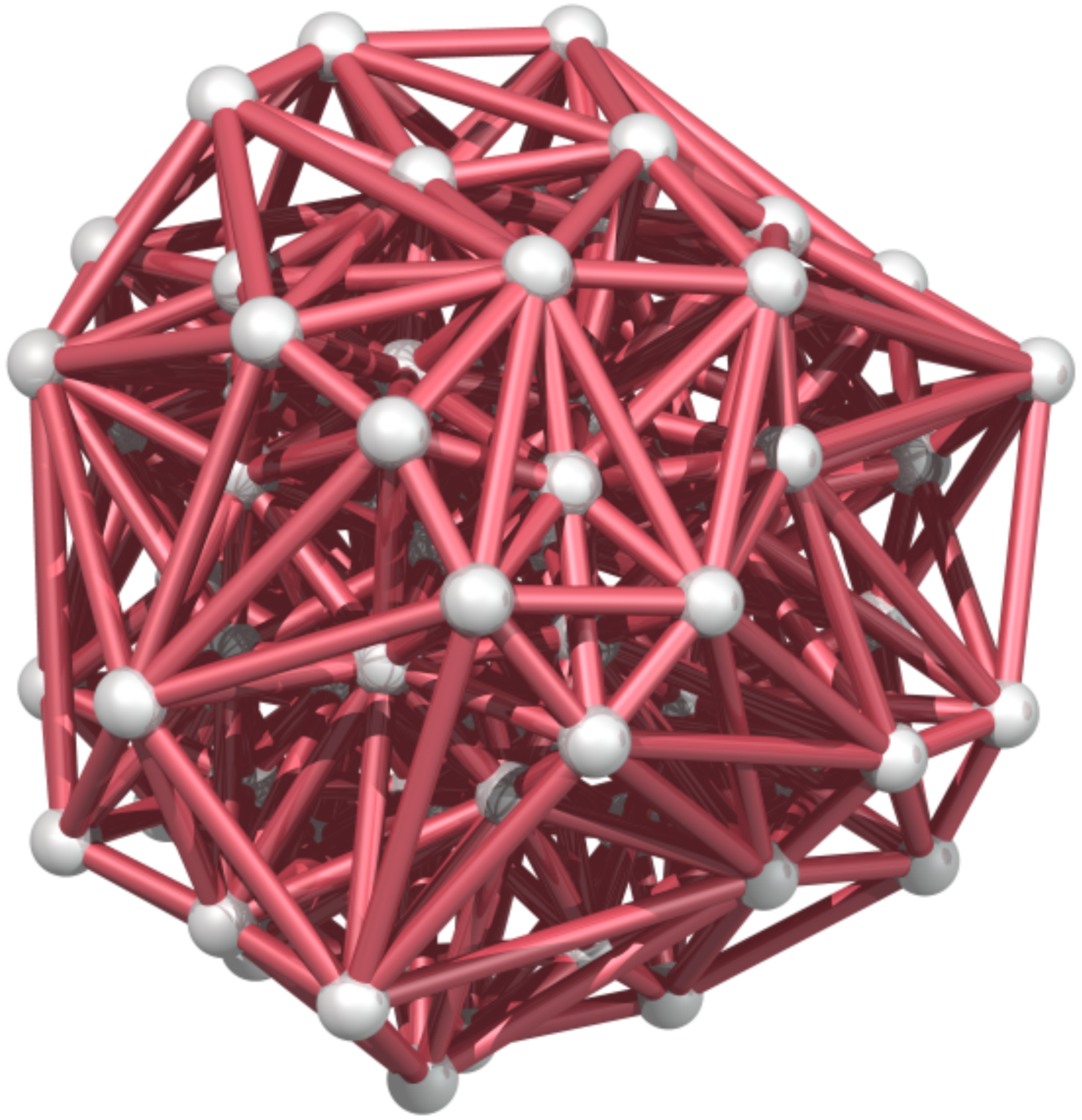
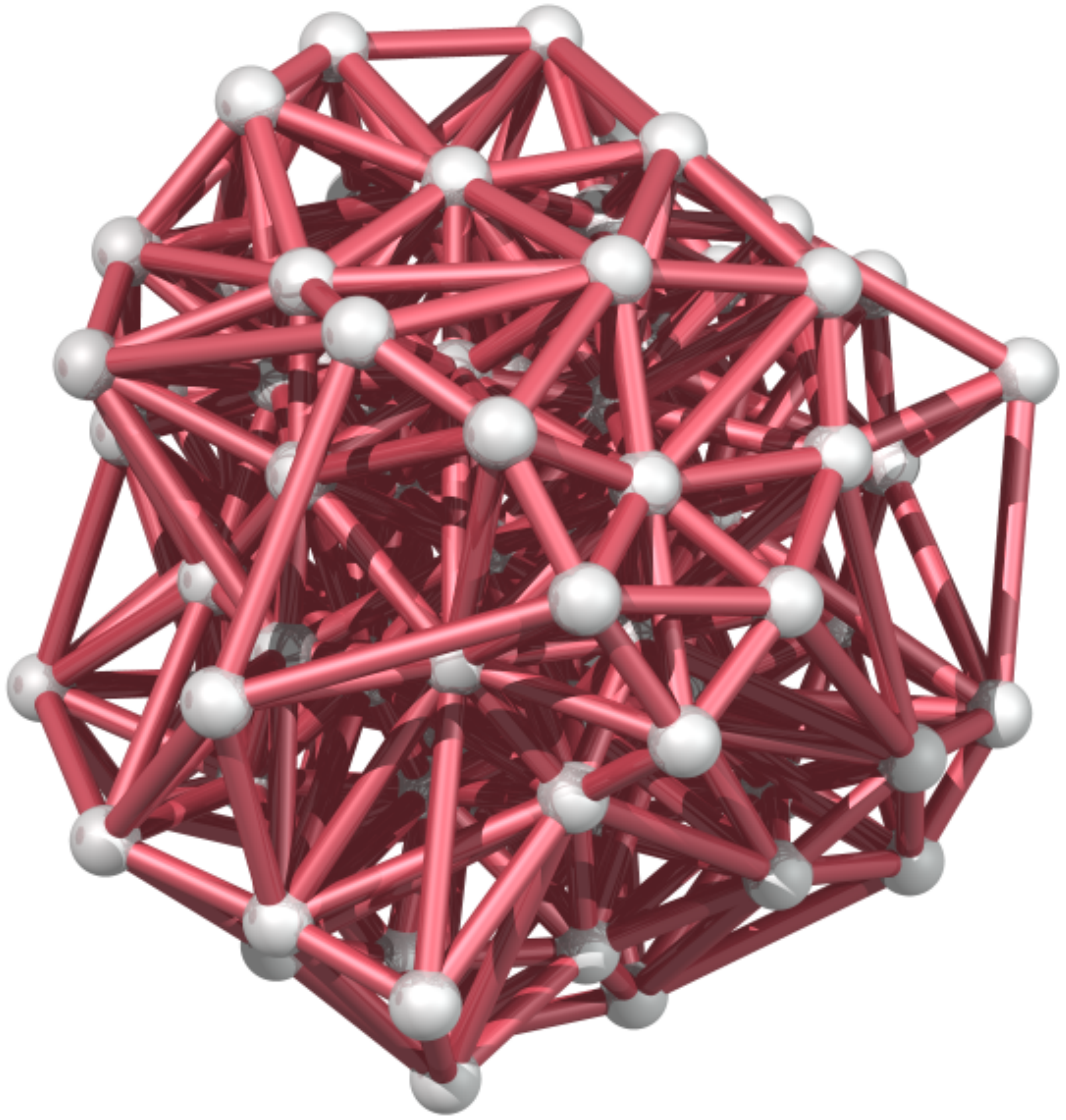
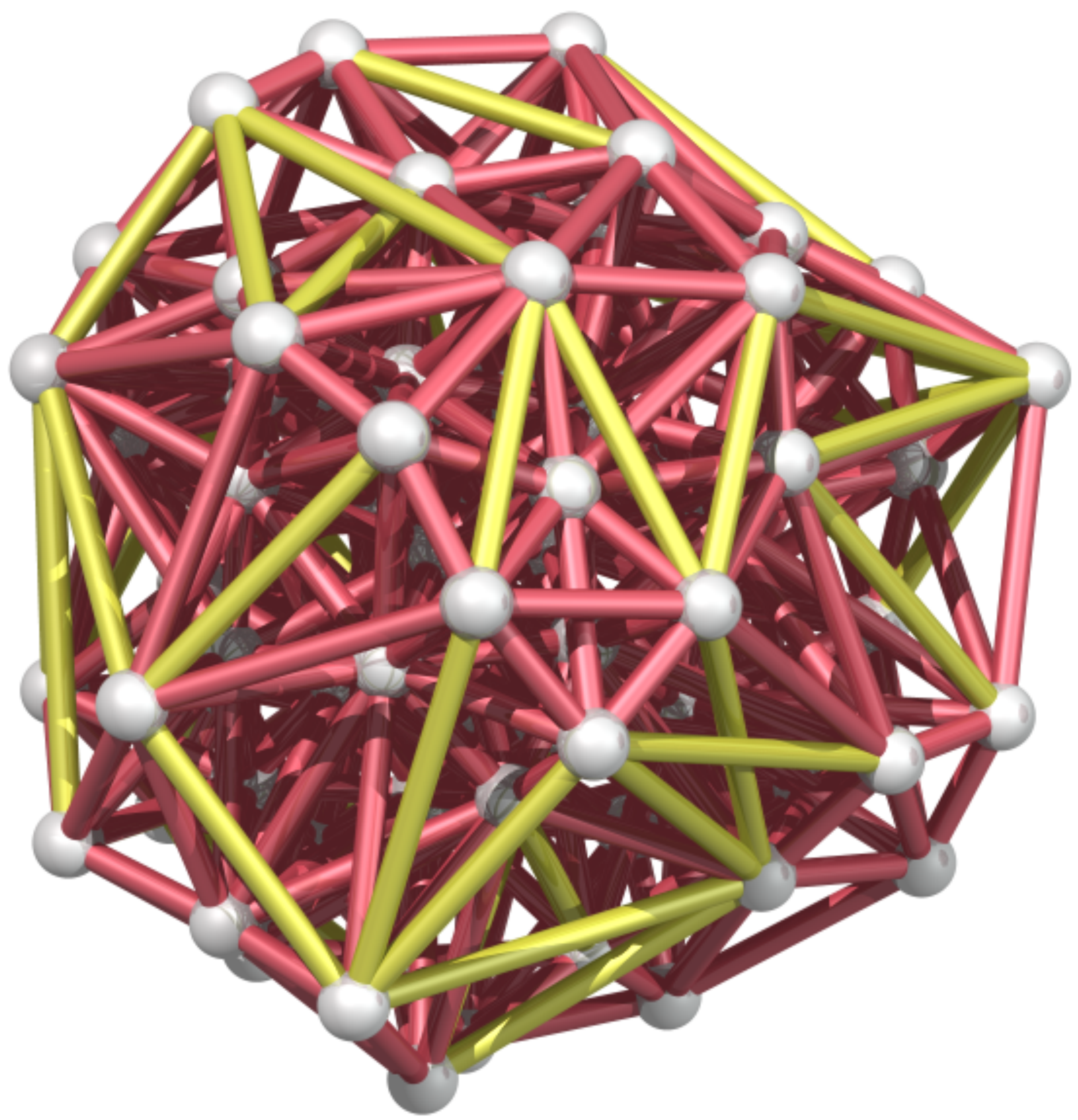


Neighbor relations from original Voronoi tessellation



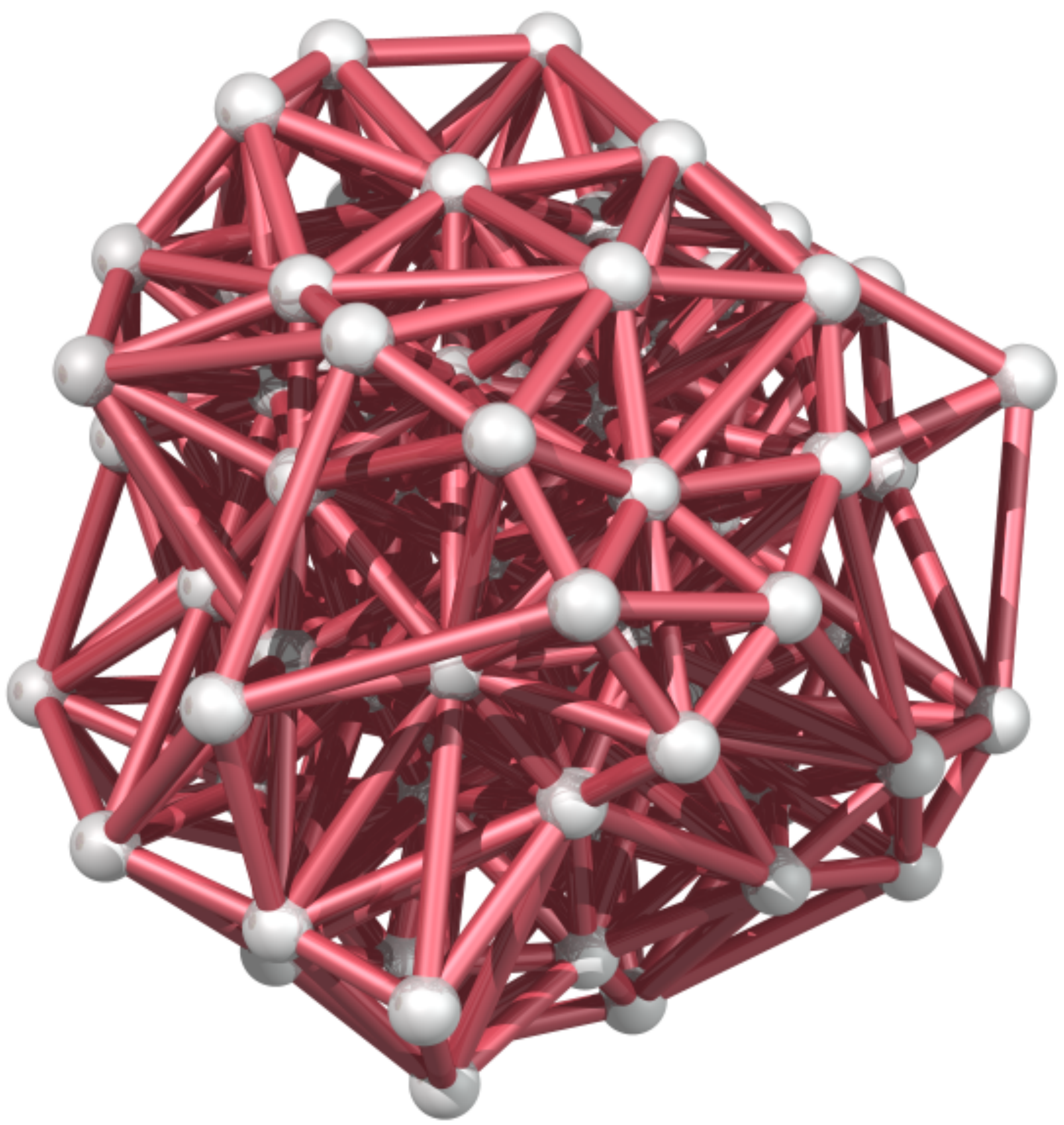
Neighbor relations from truncated Voronoi tessellation

Irregular particle packings



Neighbor relations from original Voronoi tessellation

(extra connections shown in yellow)



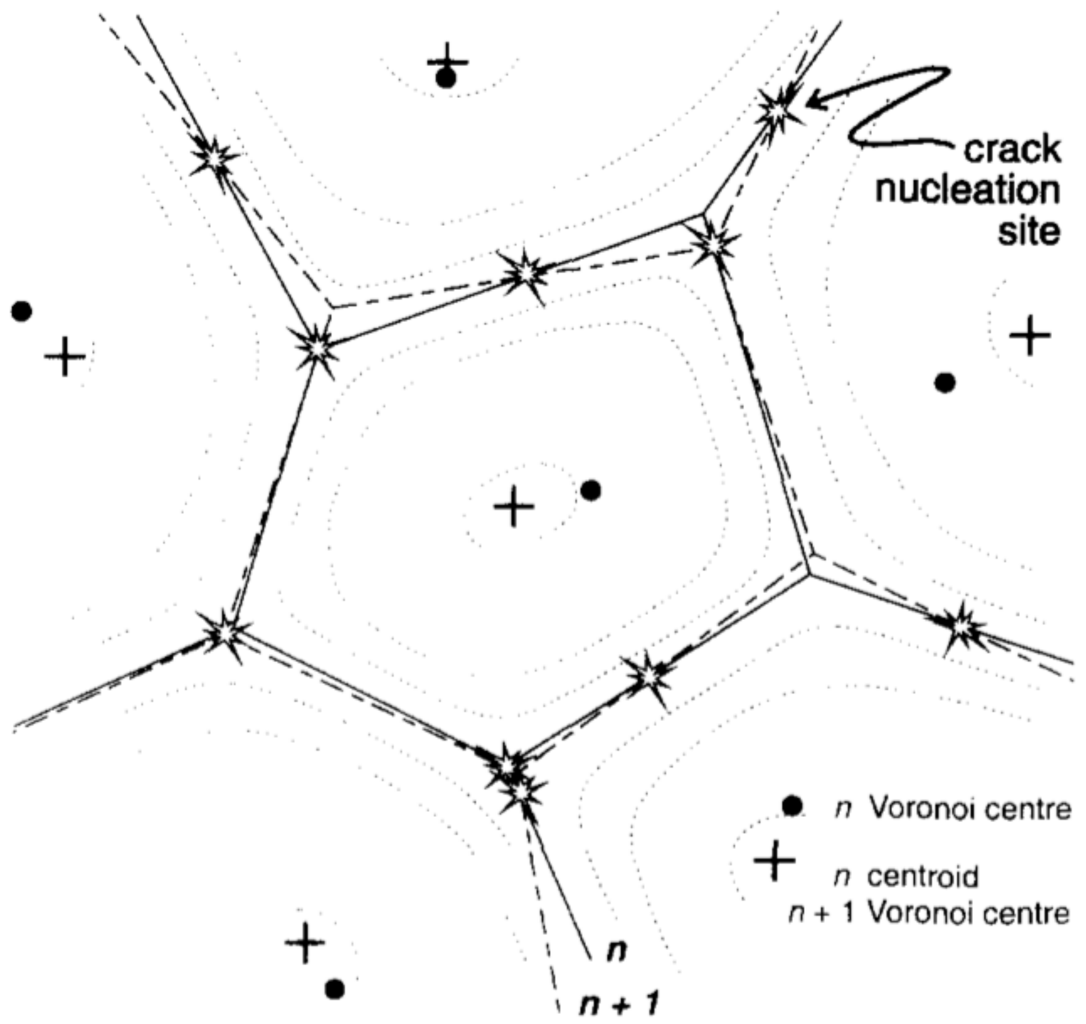
Neighbor relations from truncated Voronoi tessellation

Hospitals


Which part of the city should each hospital cover?
Voronoi tessellation minimizes distance that people must travel
Broomfield
Federal Heights
Commerce City
Wheat Ridge
Golden
Denver
Aurora
Englewood
Denver International Airport

Basalt column formation

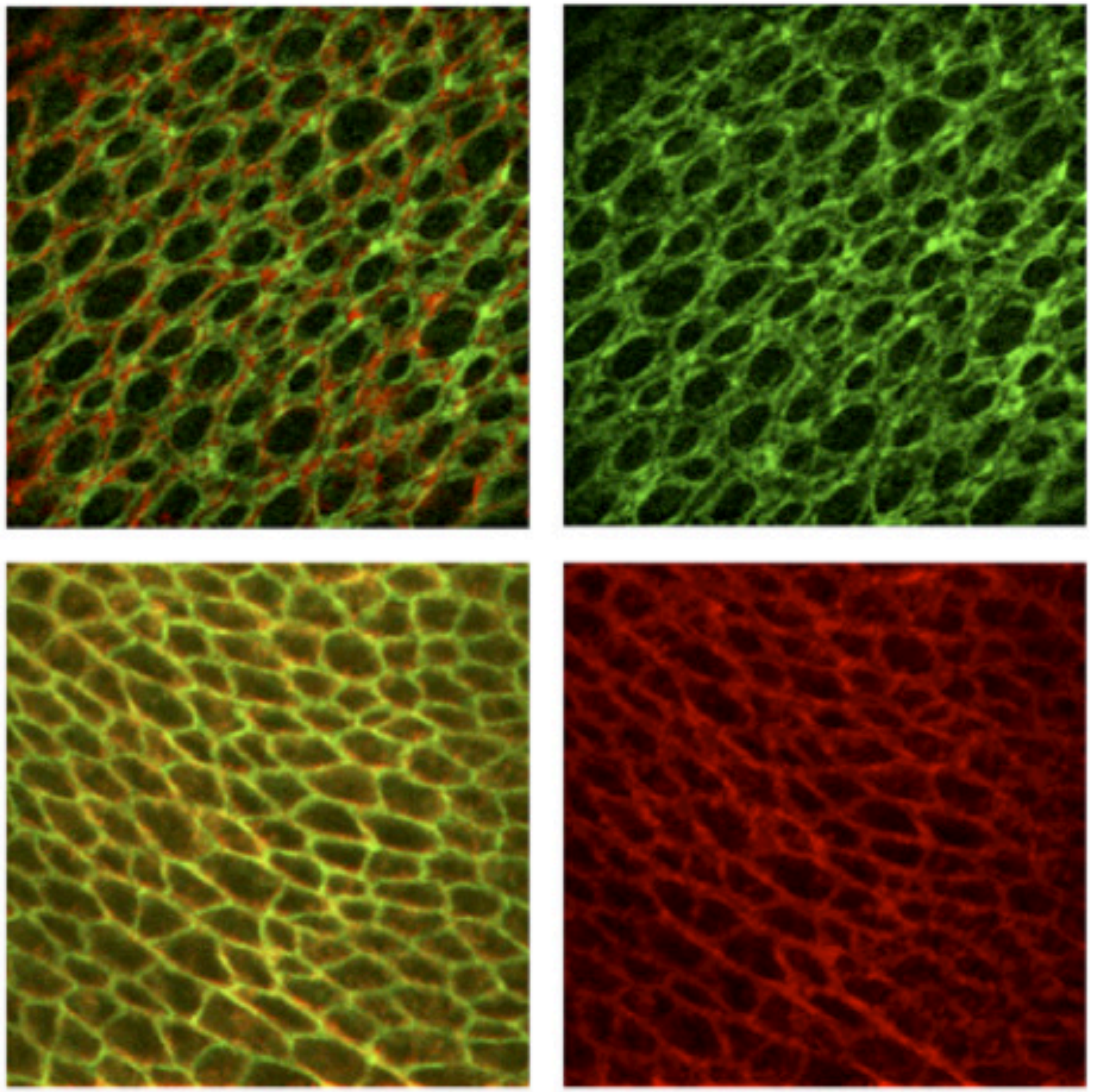
(at Giant's Causeway, Northern Ireland)



- Vertical cracks form during rapid cooling of lava
- As they extend upwards, the cracked regions become shaped more like Voronoi cells

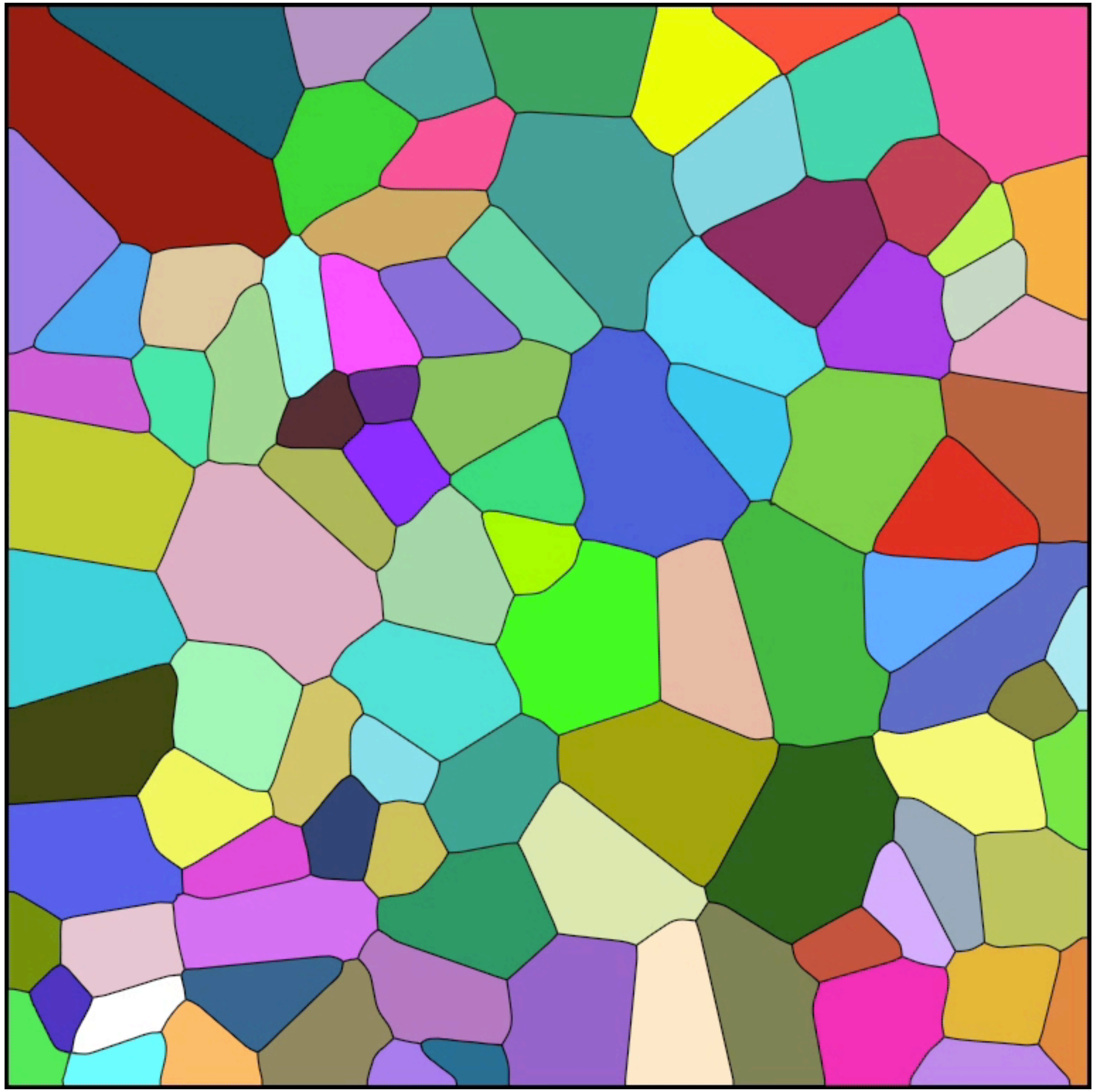
P. Budkewitsch and P.-Y. Robin, J. Volcanal. Geotherm. Res. **59**, 219–239 (1994).

Patterns in cell boundaries



Cell membranes in a fruit fly (*Drosophila*) wing

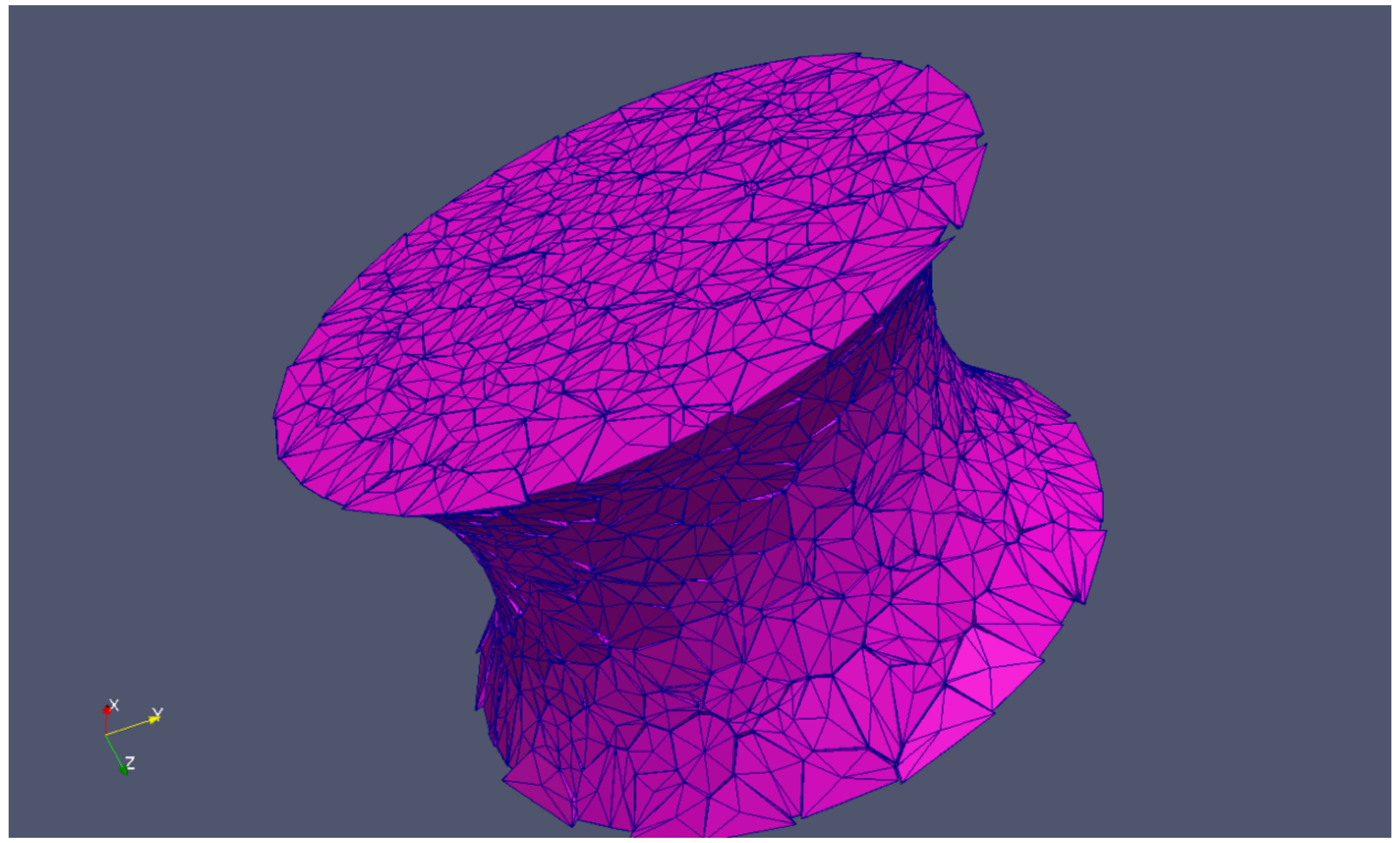
R. Farhadifar, Current Biology **17**, 2095-2104 (2007).



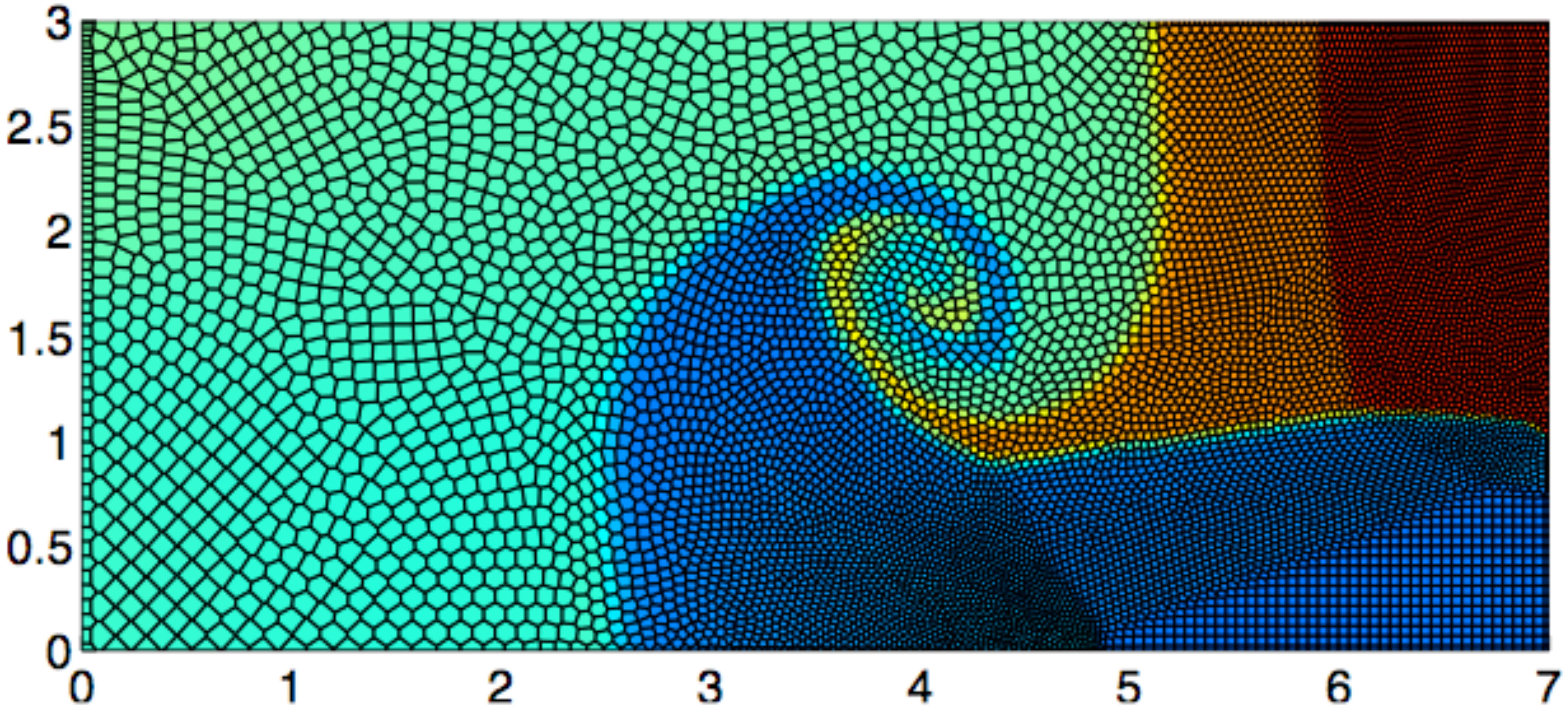
Simulation of a 2D fluid evolving under surface tension

R. Saye and J. Sethian, Proc. Natl. Acad. Sci. **105**, 907–911 (2011).

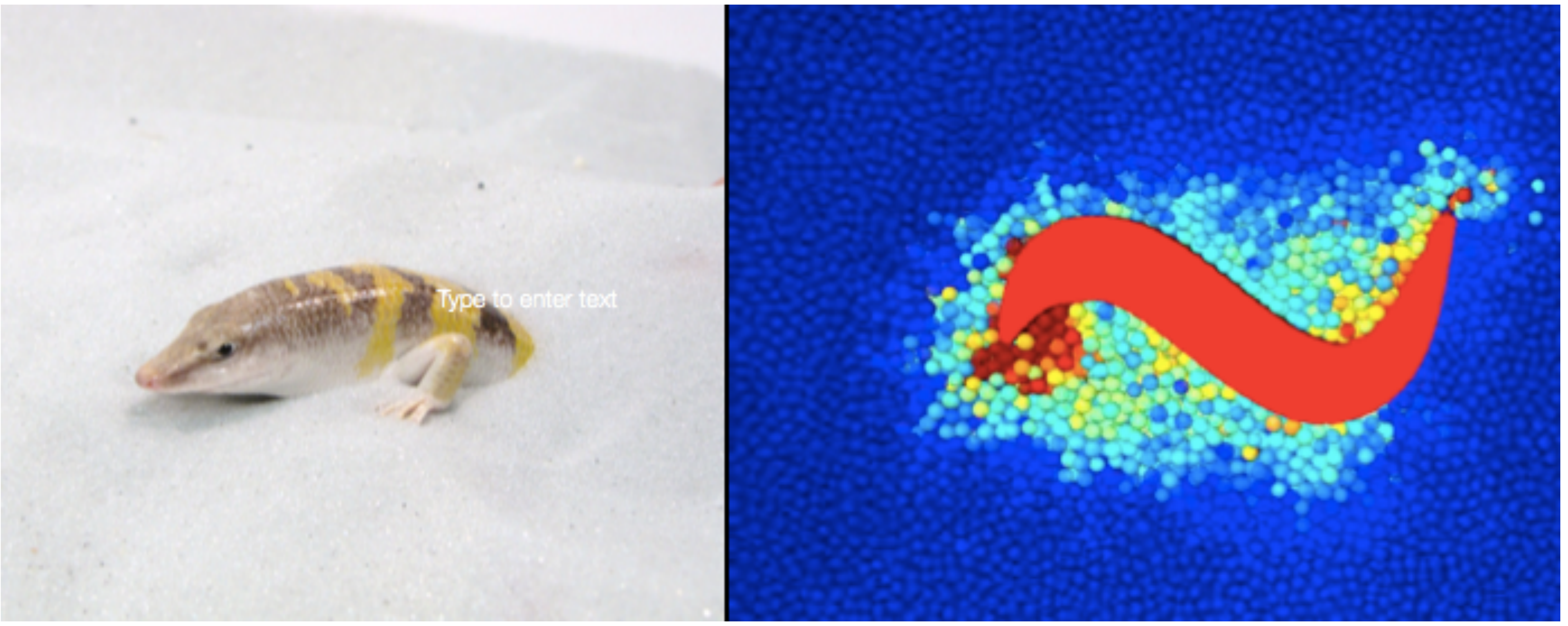
Applications of Voro++



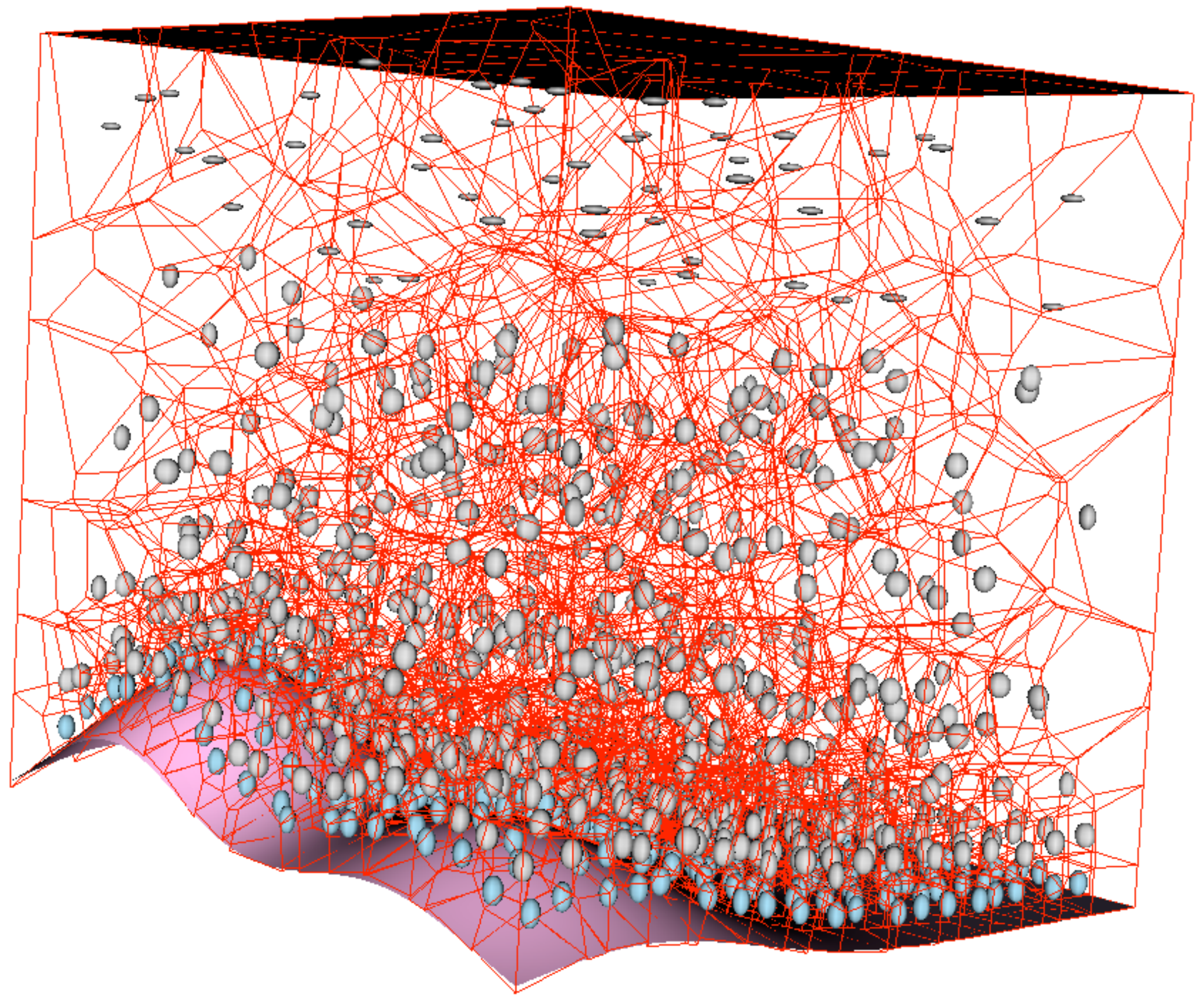
Solidification processes
(André Phillion, UBC)



Fluid simulation based upon Voronoi cells
(M. Shashkov, Los Alamos National Lab)



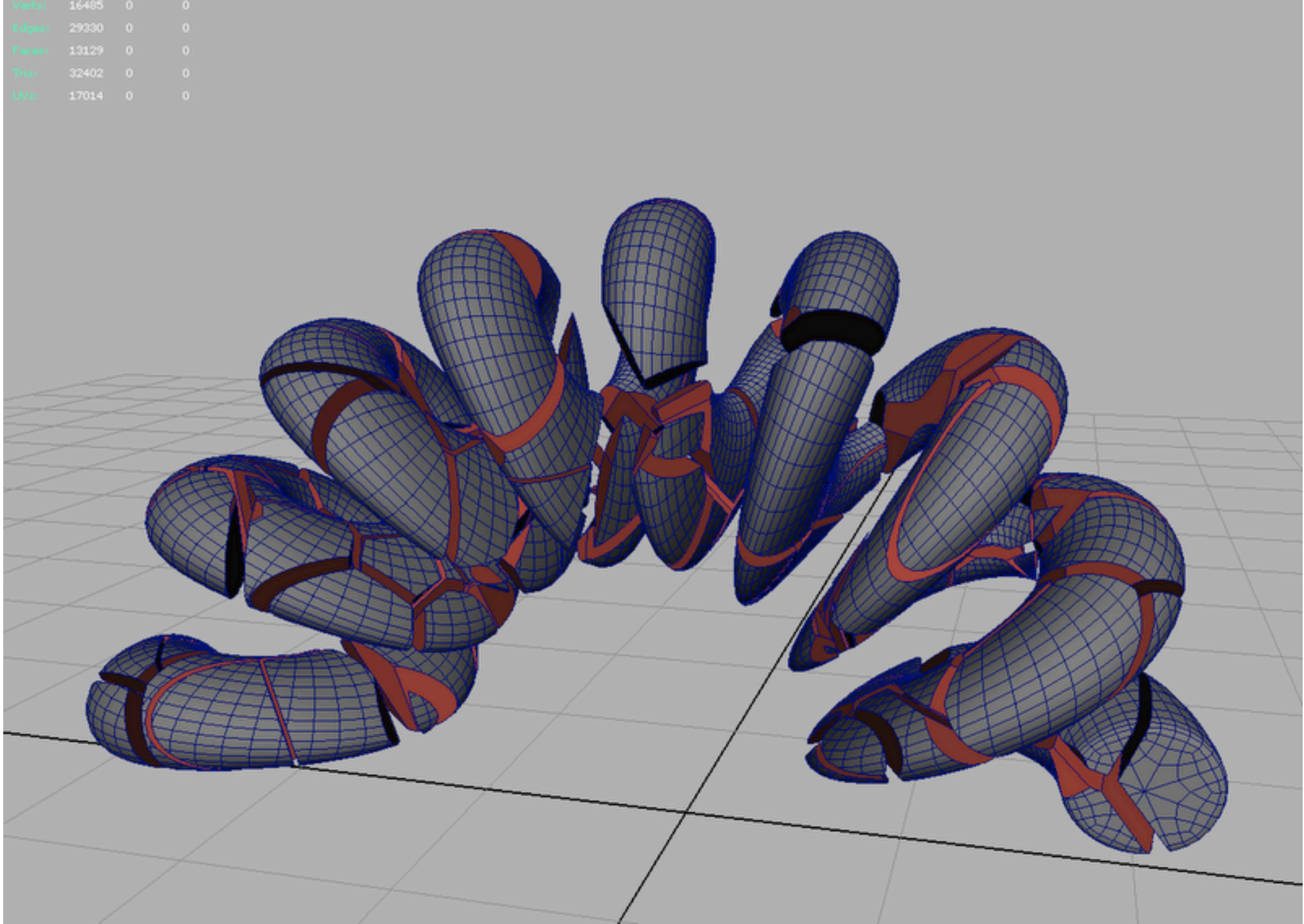
Mechanics of sand swimmers
(Goldman group, Georgia Tech)



3D biological cell boundary modeling
(M. Guillaud & L. Fenelon, BC Cancer Research Center)

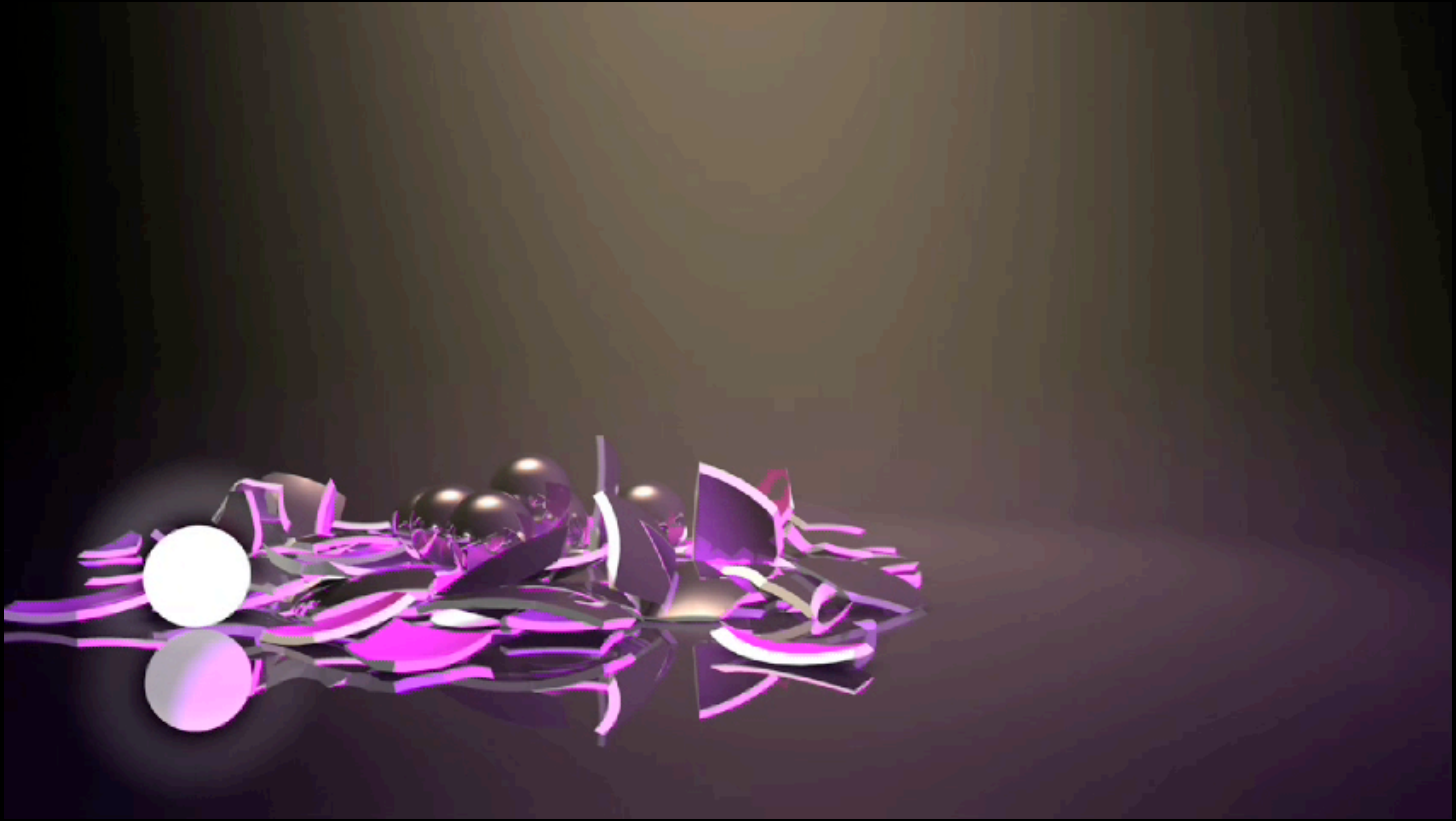
Computer graphics of object shattering

(by Dave Greenwood)



Computer graphics of object shattering

(Using Xplode plugin for Cinema4D, by Manuel Magalhaes)



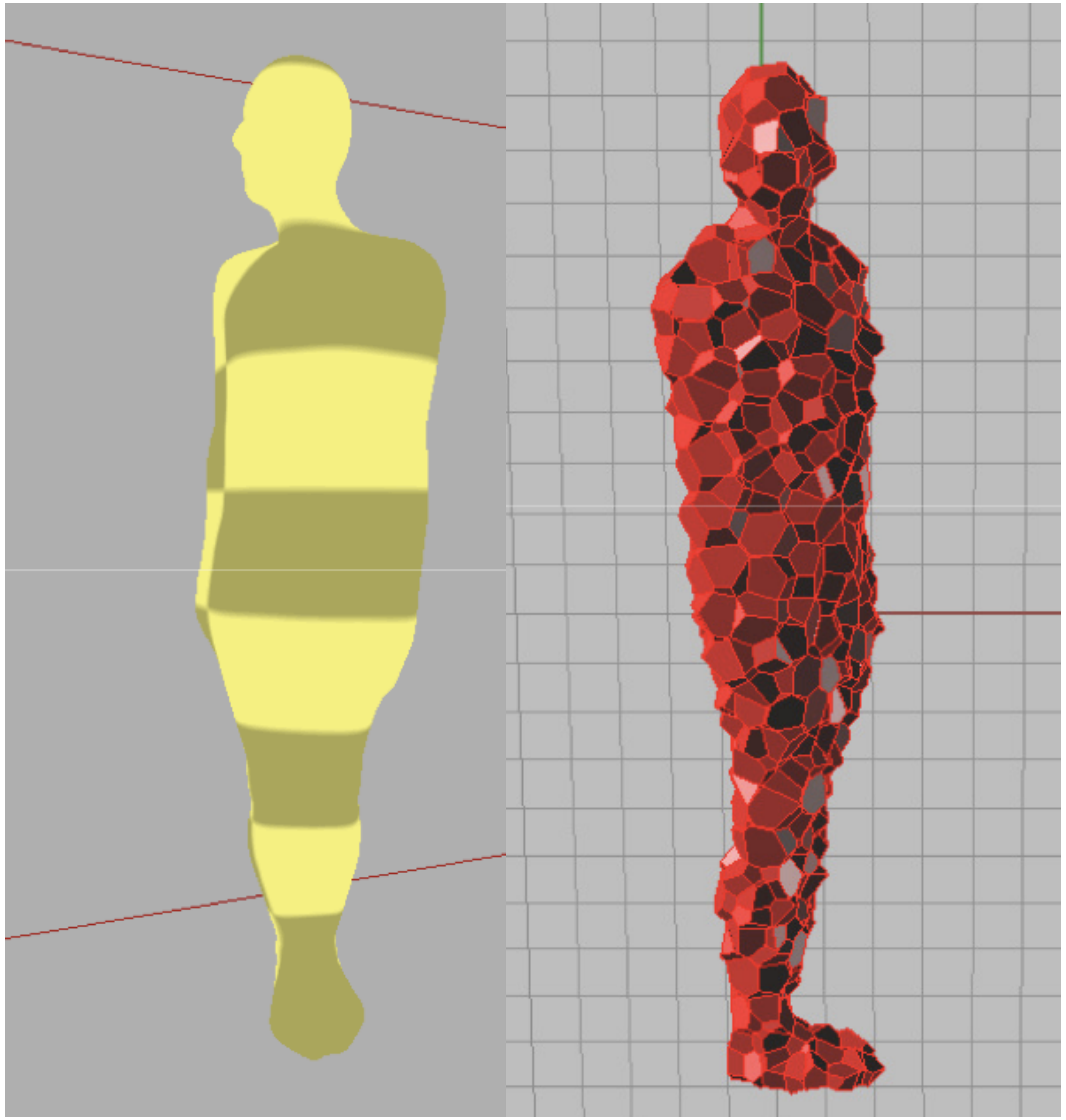
http://xplode.valkaari.com/en/xplode.php

Voronoi-based sculptures

The Angel of the North,
by Antony Gormley (1998)
(Near Newcastle, England)

Another Place (2005)

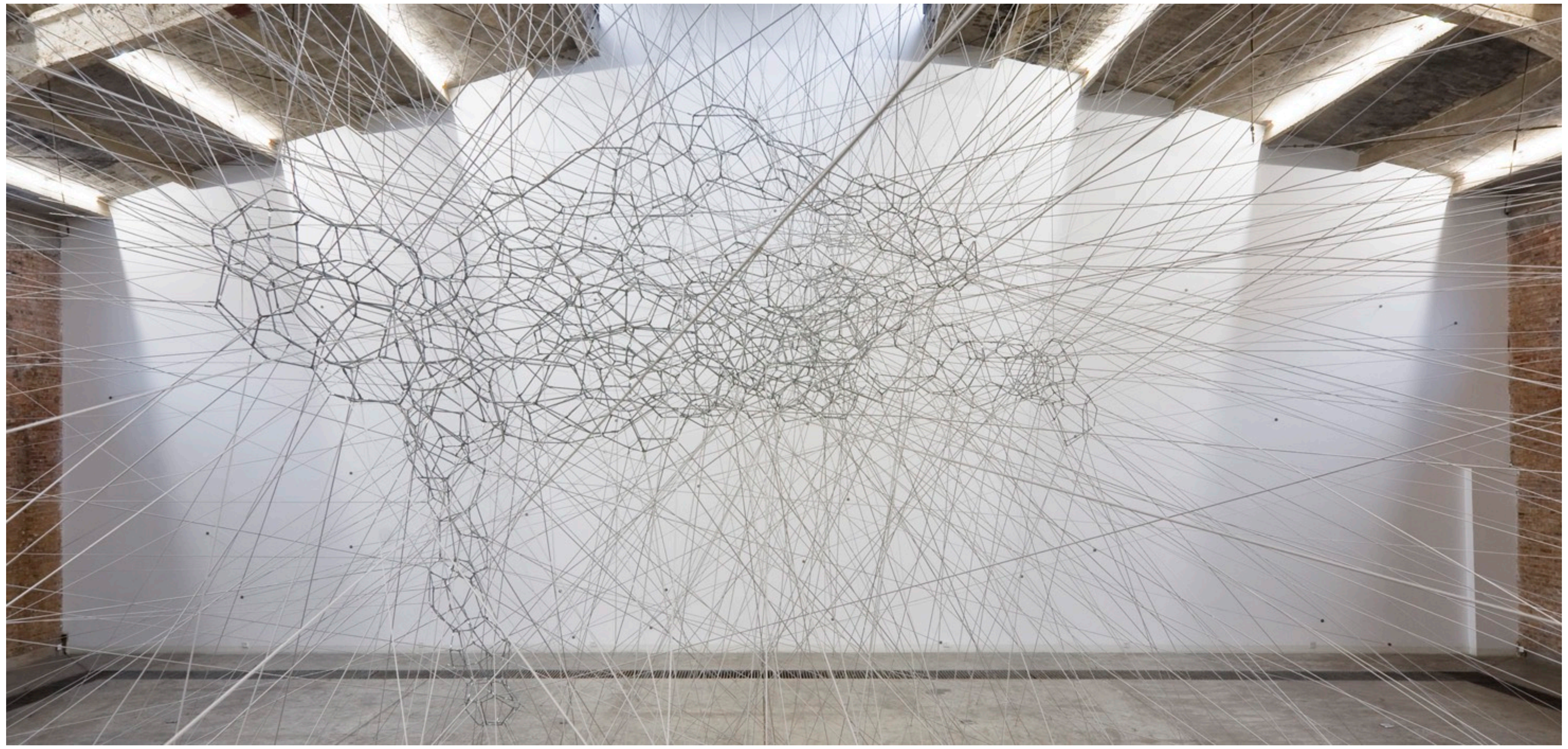
Event Horizon (2010)



Voronoi-based sculpture
(T. Simmonds, Antony Gormley studio, London)

Sculptures based on Voronoi cells

(from www.antonygormley.com)



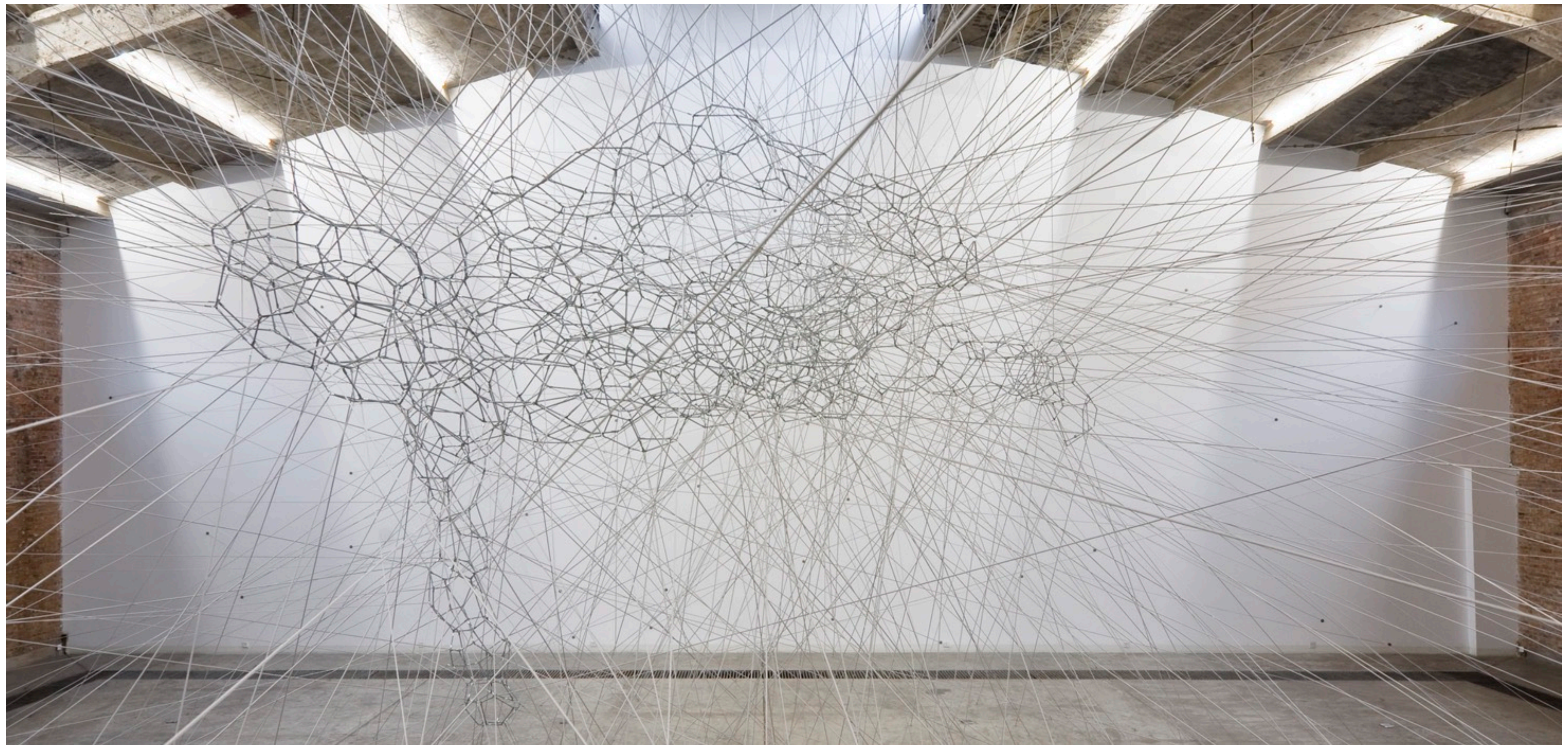
Fuse, 2011

Another Singularity (China), 2009

Chord (MIT Mathematics), 2016

Sculptures based on Voronoi cells

(from www.antonygormley.com)



Fuse, 2011

Chord (MIT Mathematics), 2016

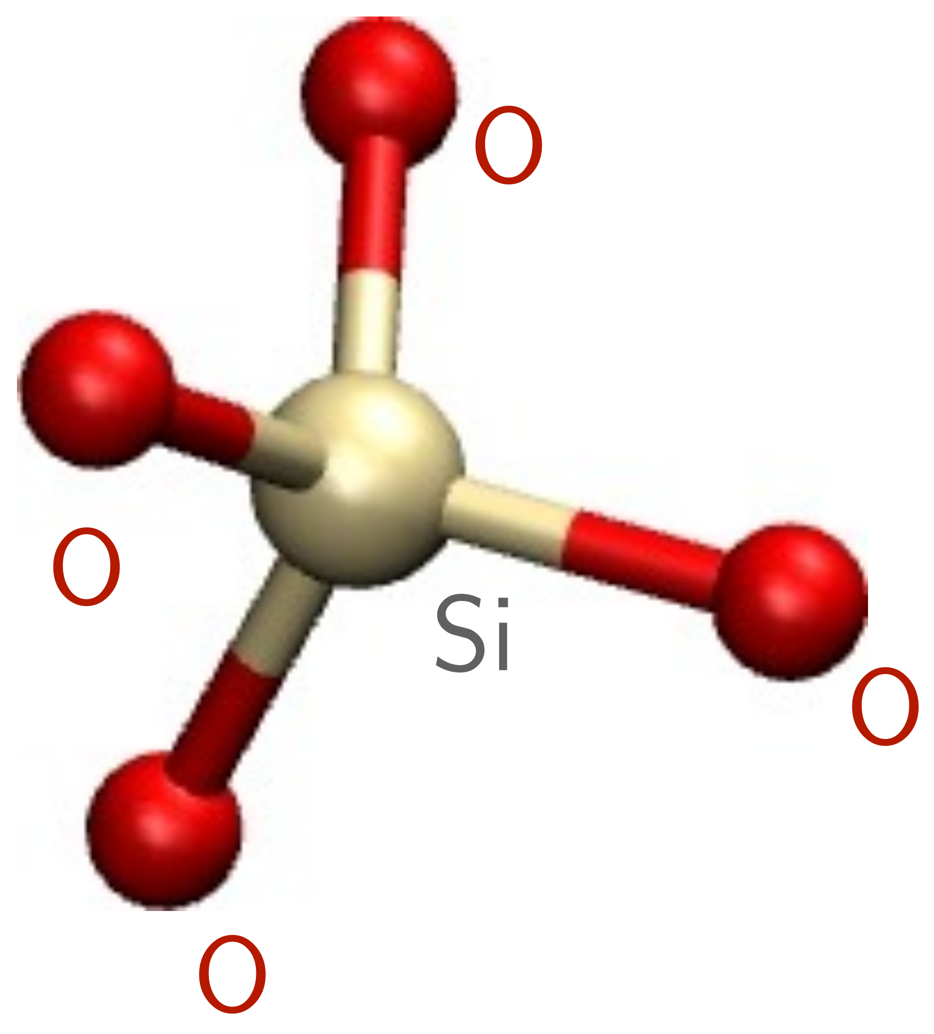
Chord (MIT Mathematics), 2016

Chord (MIT Mathematics), 2016

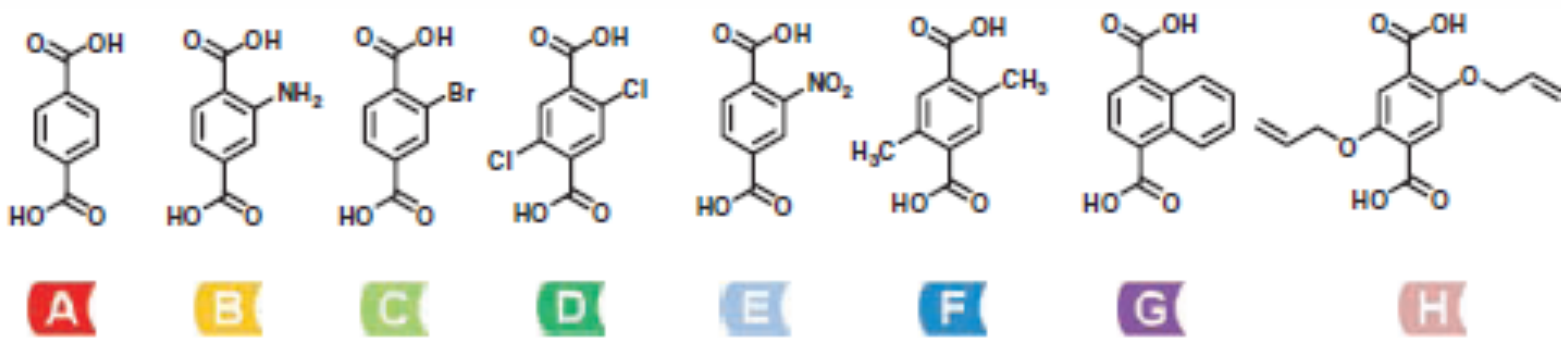
Crystalline porous materials

Zeolites

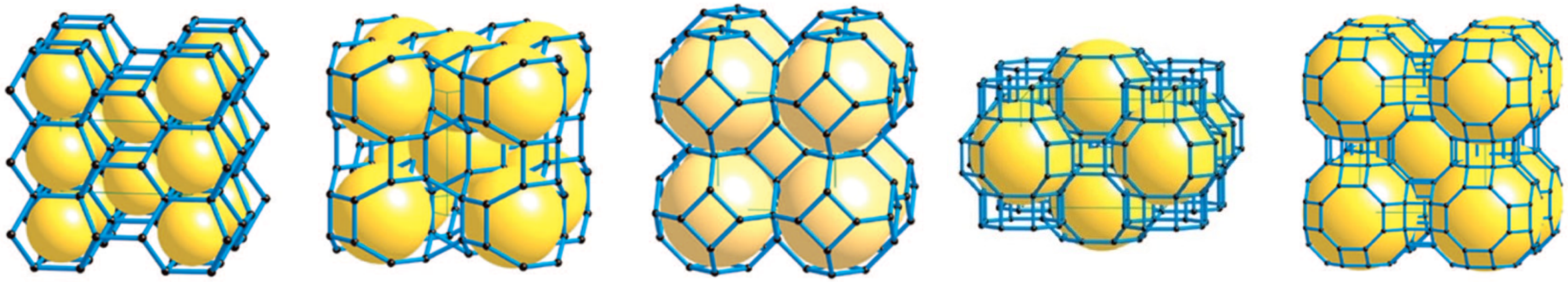
- Composed of tetrahedral building blocks of atoms
- 190 known structures, but millions of hypothetical ones



Metal organic frameworks



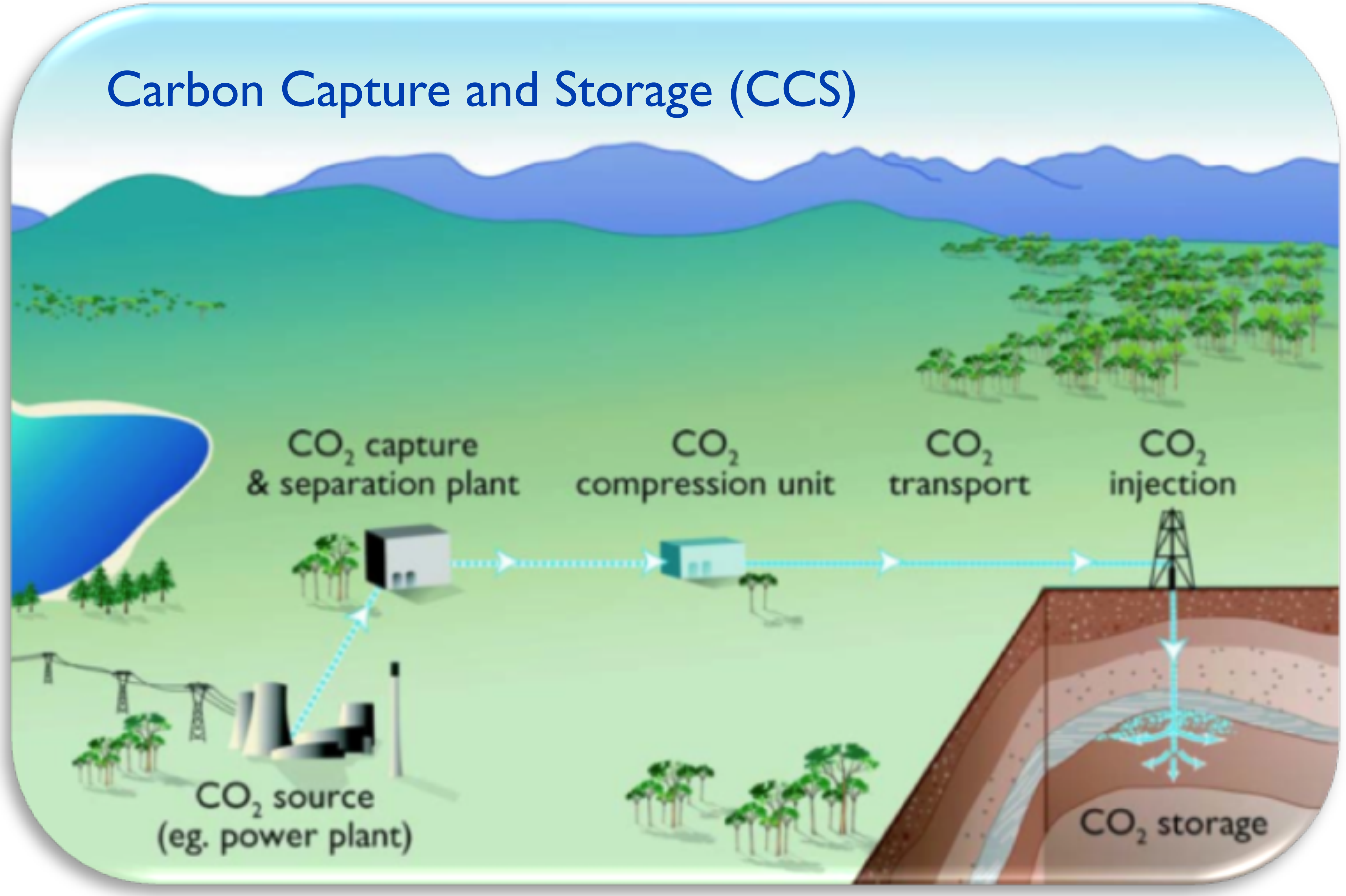
- Composed of building blocks with metallic centers
- Even more potential structures than zeolites, with thousand per year synthesized



Many different topologies (yellow represents void space)

Applications of porous materials

- Zeolites very important in many industrial processes
- Market of $350 billion a year for catalysts in petroleum refining, and detergents
- Other applications include refrigeration, reprocessing, construction, agriculture
- Current carbon capture technology relies on scrubbing gases with amine solutions and requires 35% of energy

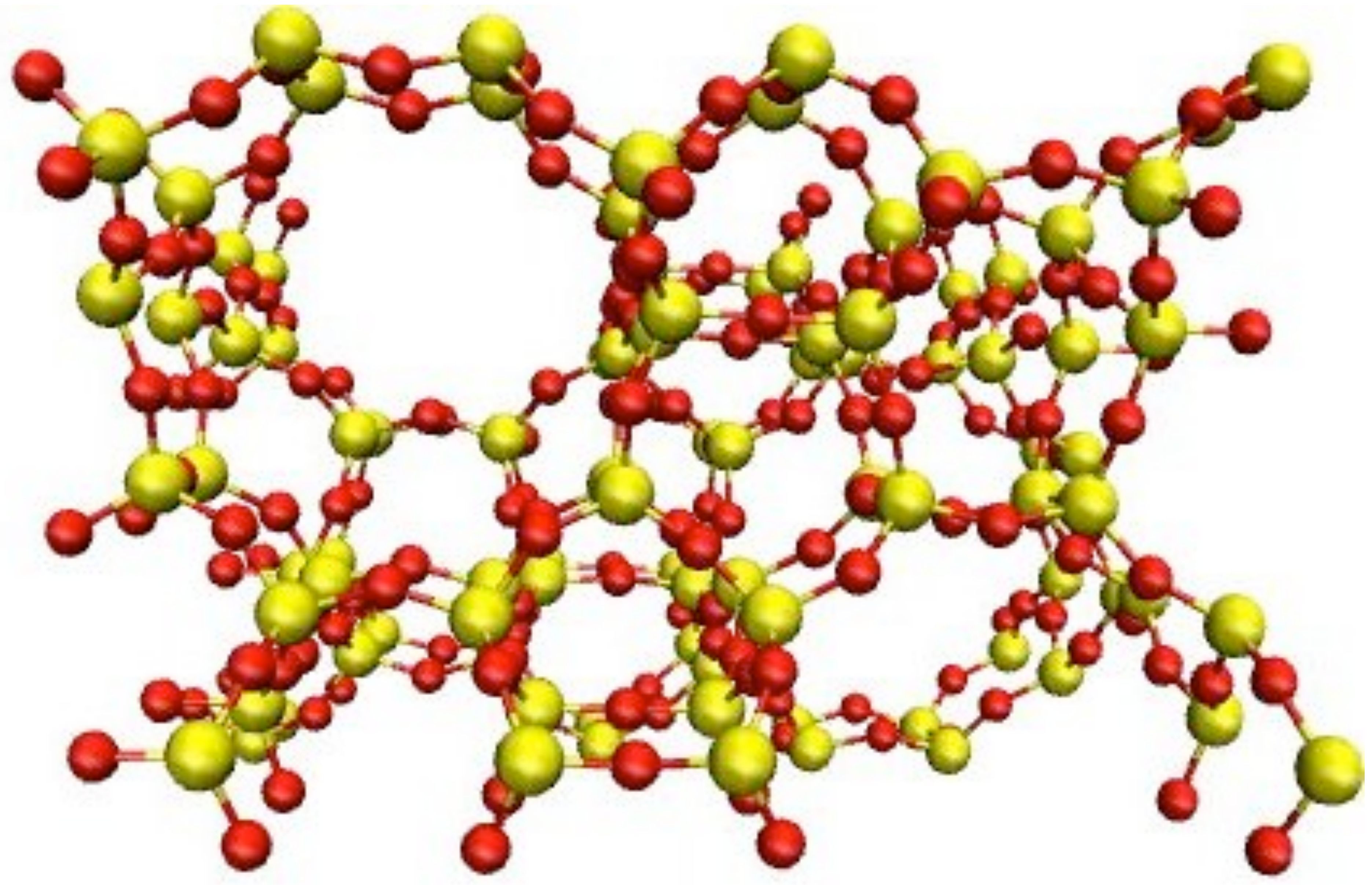


- Using porous materials as adsorbents is a promising alternative

Phan *et al.*, Acc. Chem. Res. **43**, 58–67 (2010).

Pore topology and screening

- For a particular application, important to select a material with a specific void topology corresponding to molecules of interest
- Numerous databases of chemical structures available:
  - IZA database of 194 known frameworks
  - 2.7 M hypothetical zeolites
  - 500,000 MOFs; many more feasible
- Specified as up to several thousand atoms in periodic unit cells



Unit cell of "MFI" zeolite

Aim: develop computational tools for high-throughput screening of chemical databases to identify structures for further study

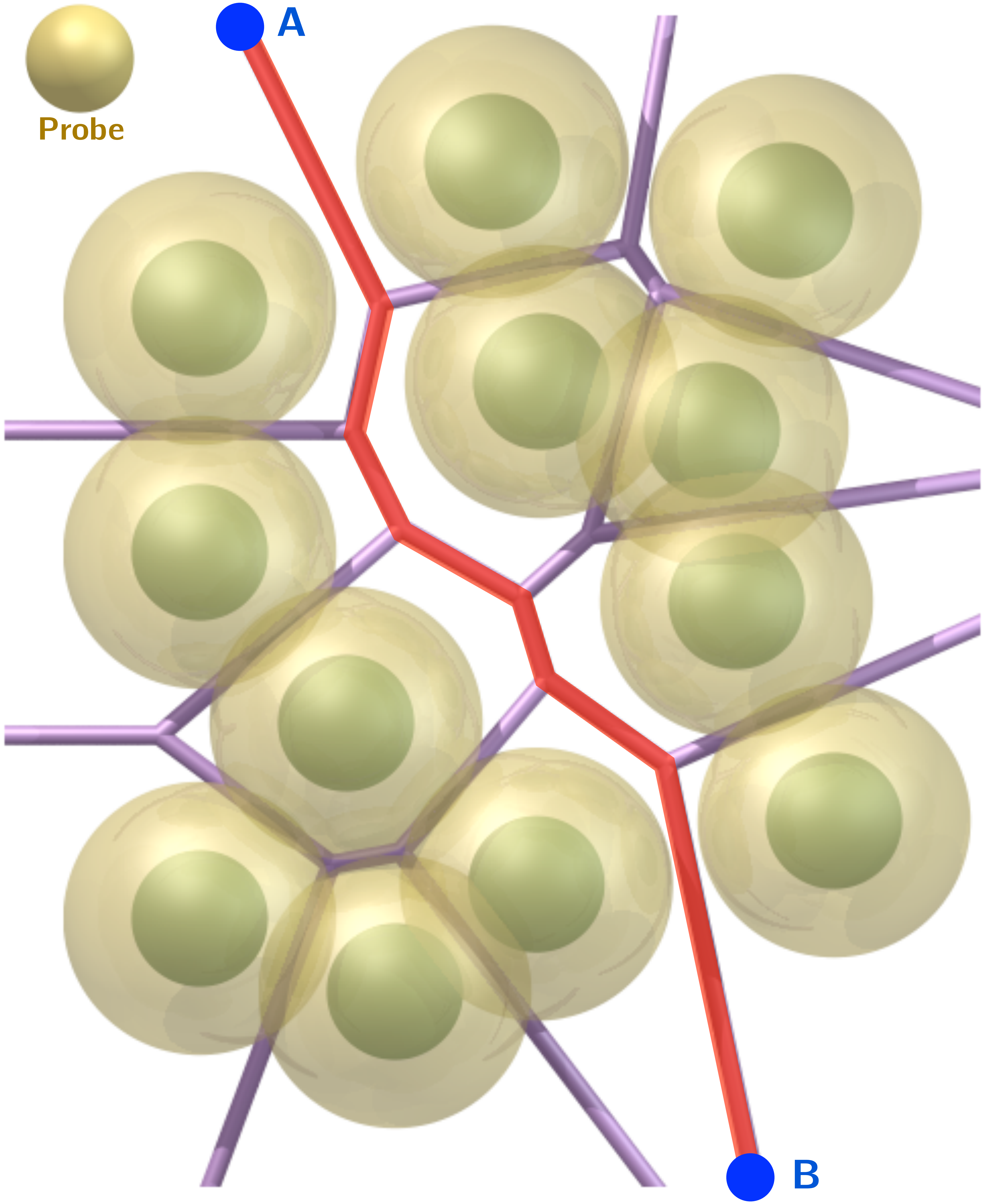
http://www.iza-structure.org/databases/

Void space analysis via the Voronoi tessellation

- Recall the Voronoi tessellation definition: for a group of points in a domain, the Voronoi cell for particle i is the space $\mathbf{x}$ closer to i than any other:

$$d(\mathbf{x}, \mathbf{x}_i) < d(\mathbf{x}, \mathbf{x}_j) \text{ for all } j \neq i$$

- Provides a map of the void space in a material, accessible to a spherical probe of a given radius



Mathematical path proble

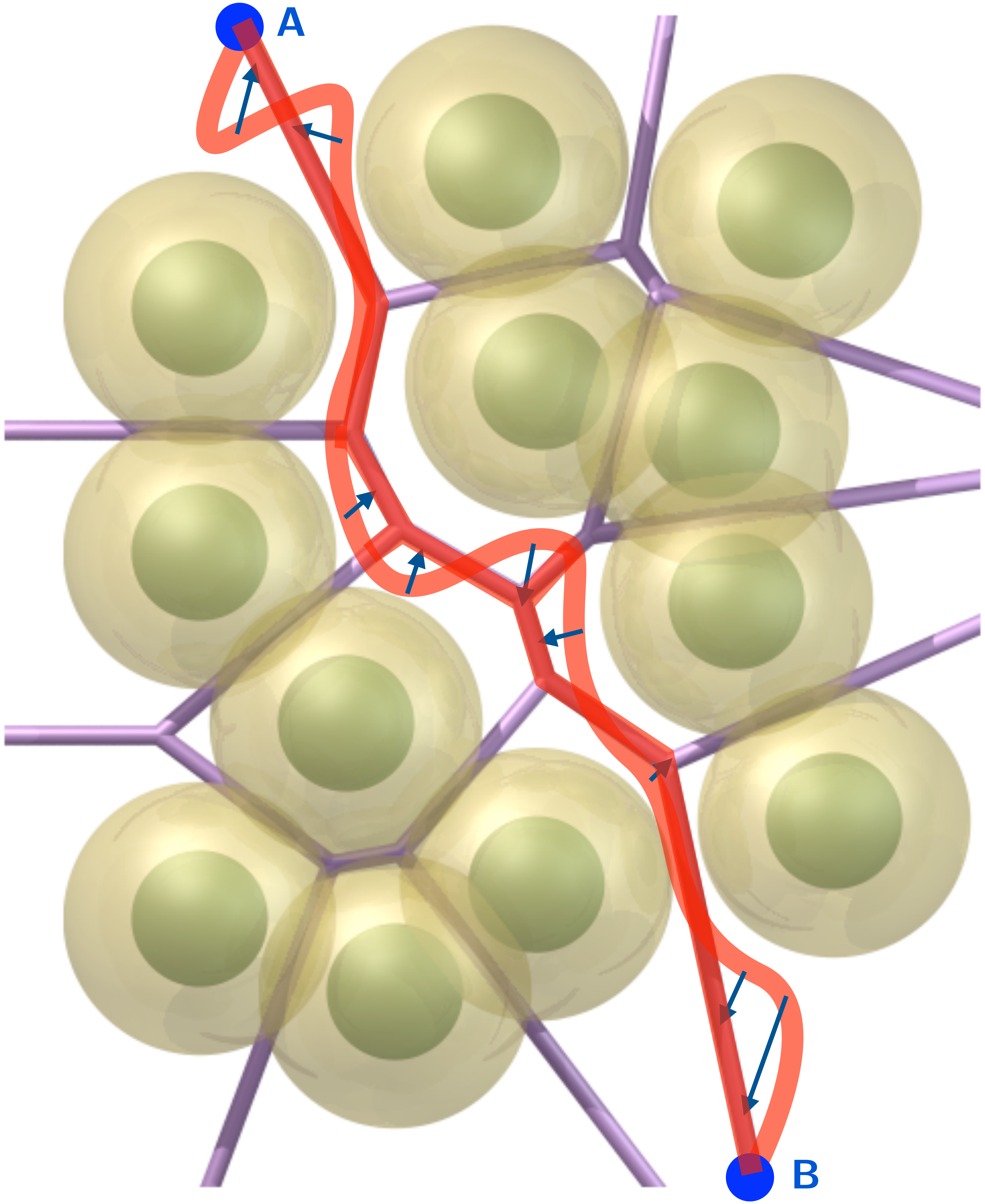
- It is clear that

Path exists from A to B on Voronoi network $\Rightarrow$ Continuous path exists between A and B

- What about the converse?

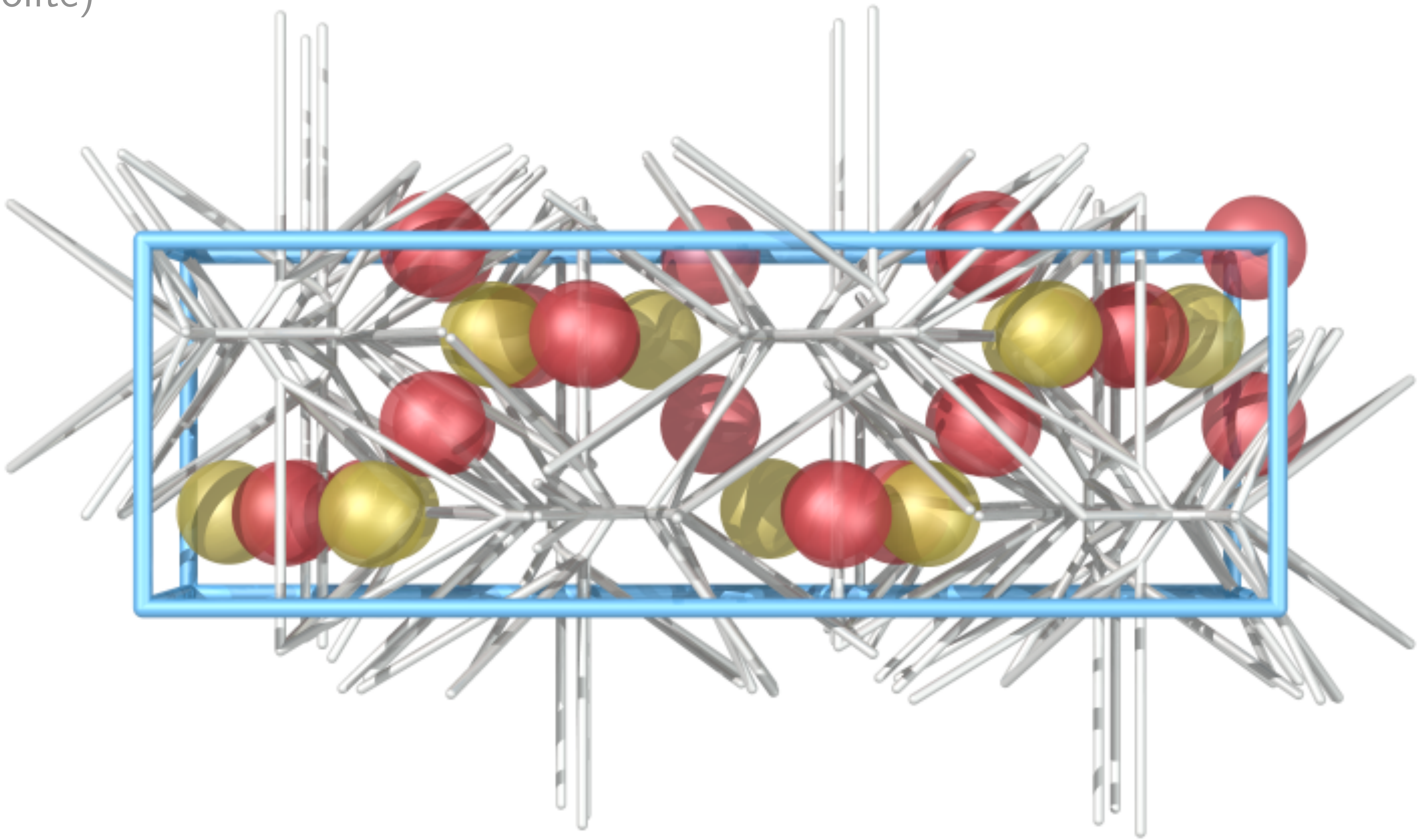
Path exists from A to B on Voronoi network $\Leftarrow$ Continuous path exists between A and B

- Can be shown by projecting continuous path radially outwards



Example computation

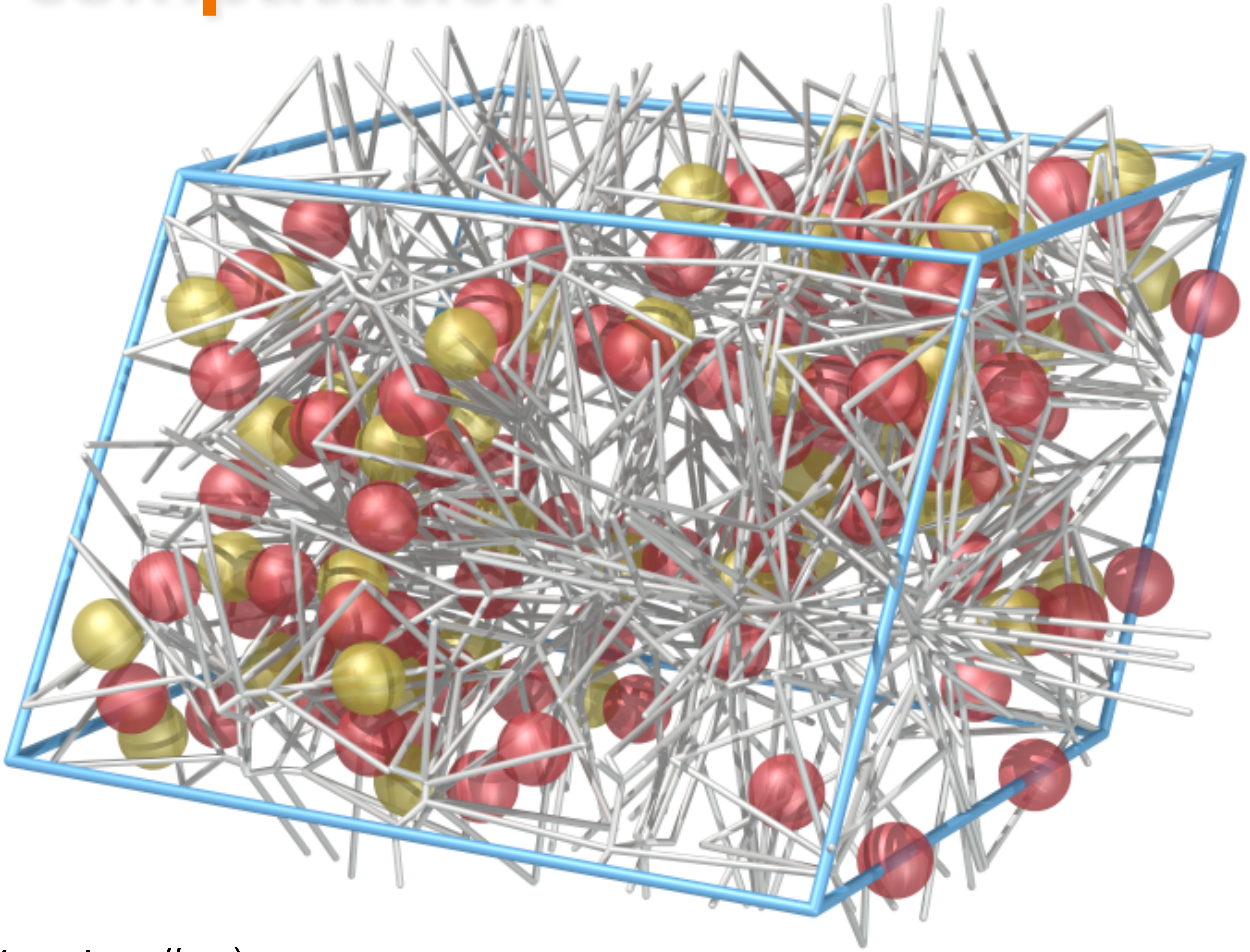
(for the BIK zeolite)



(Oxygen atoms in red, silicon in yellow)

Example computation

(for the AFX zeolite)



(Oxygen atoms in red, silicon in yellow)