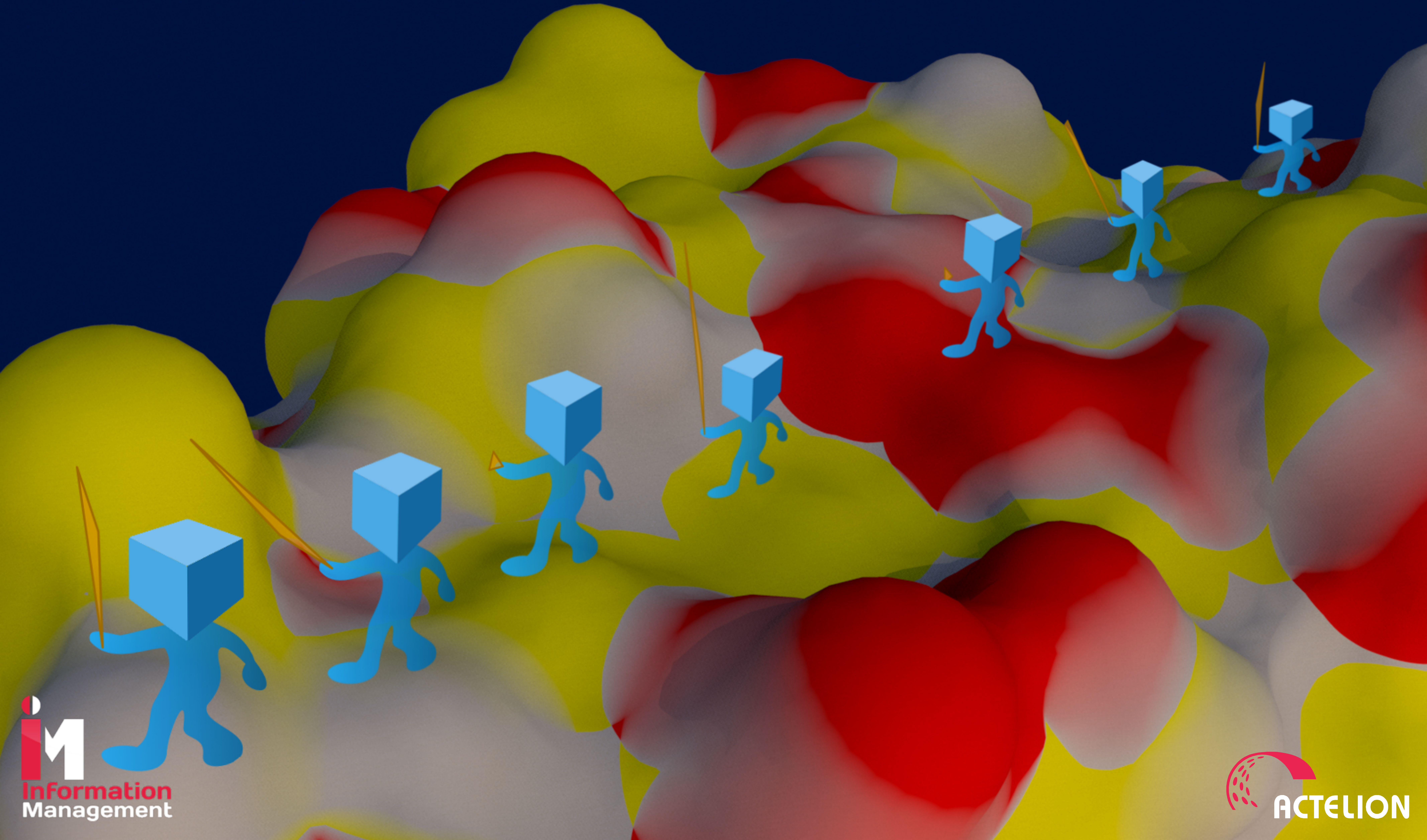
Marching Cubes Without Skinny And Tiny Triangles

And How To Employ Them To Create Smooth Molecular Surfaces

Thomas Sander, Sep 2016



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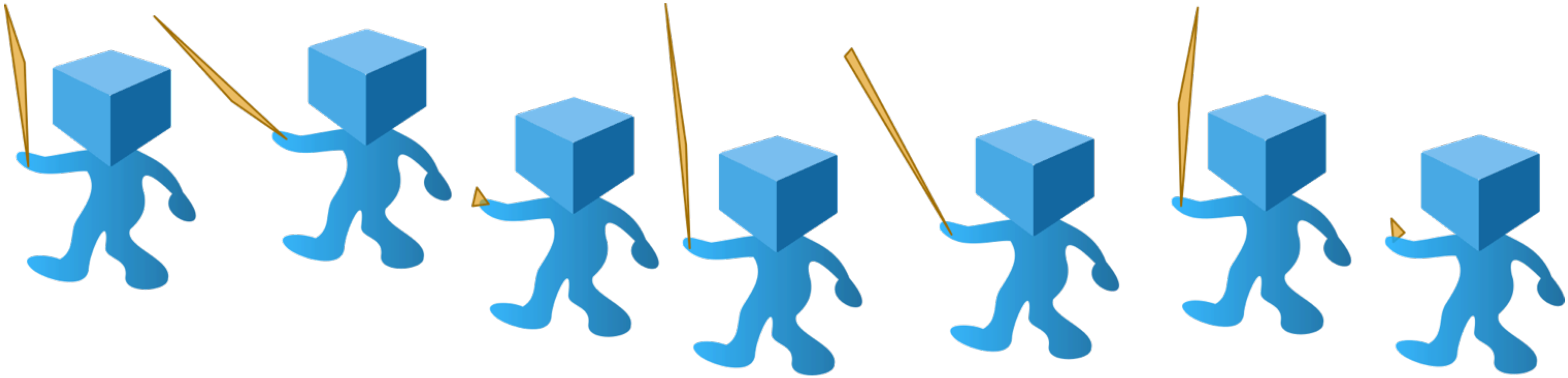
- What are Marching Cubes?

- Why do we care about them?

- Why do they carry small and skinny triangles?

- How to make them relinquish these triangles?



The Marching Cubes Algorithm

Iso-Layer Triangulation from Voxel Data

- Paper published in the 1987 SIGGRAPH

  Lorensen, W. E.; Cline, Harvey E. (1987). "Marching cubes: A high resolution 3d surface construction algorithm". ACM Computer Graphics. 21 (4): 163–169.

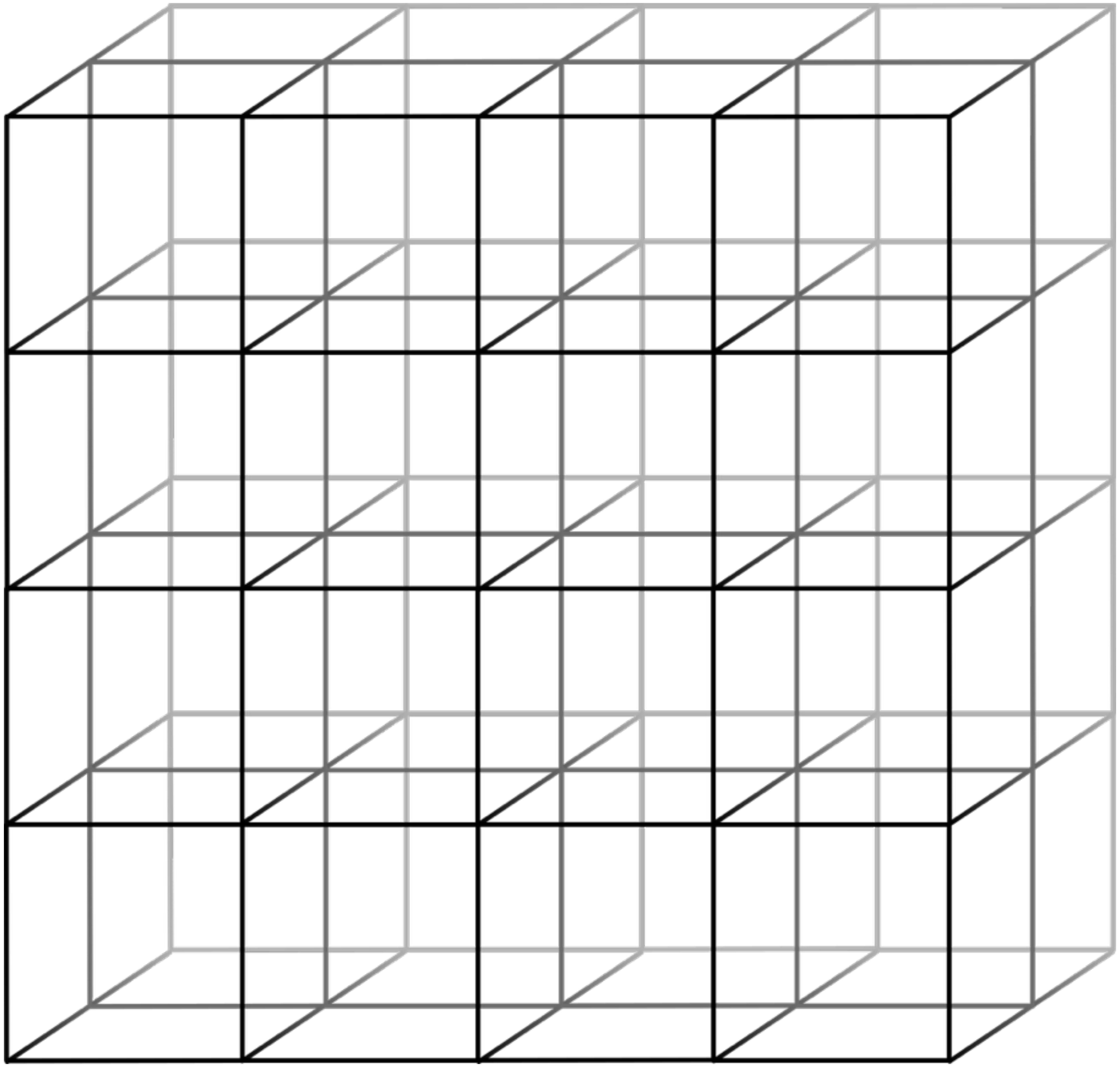
  DOI: 10.1145/37402.37422

- One of the most frequently cited papers in computer graphics field

- Patent expired in 2005

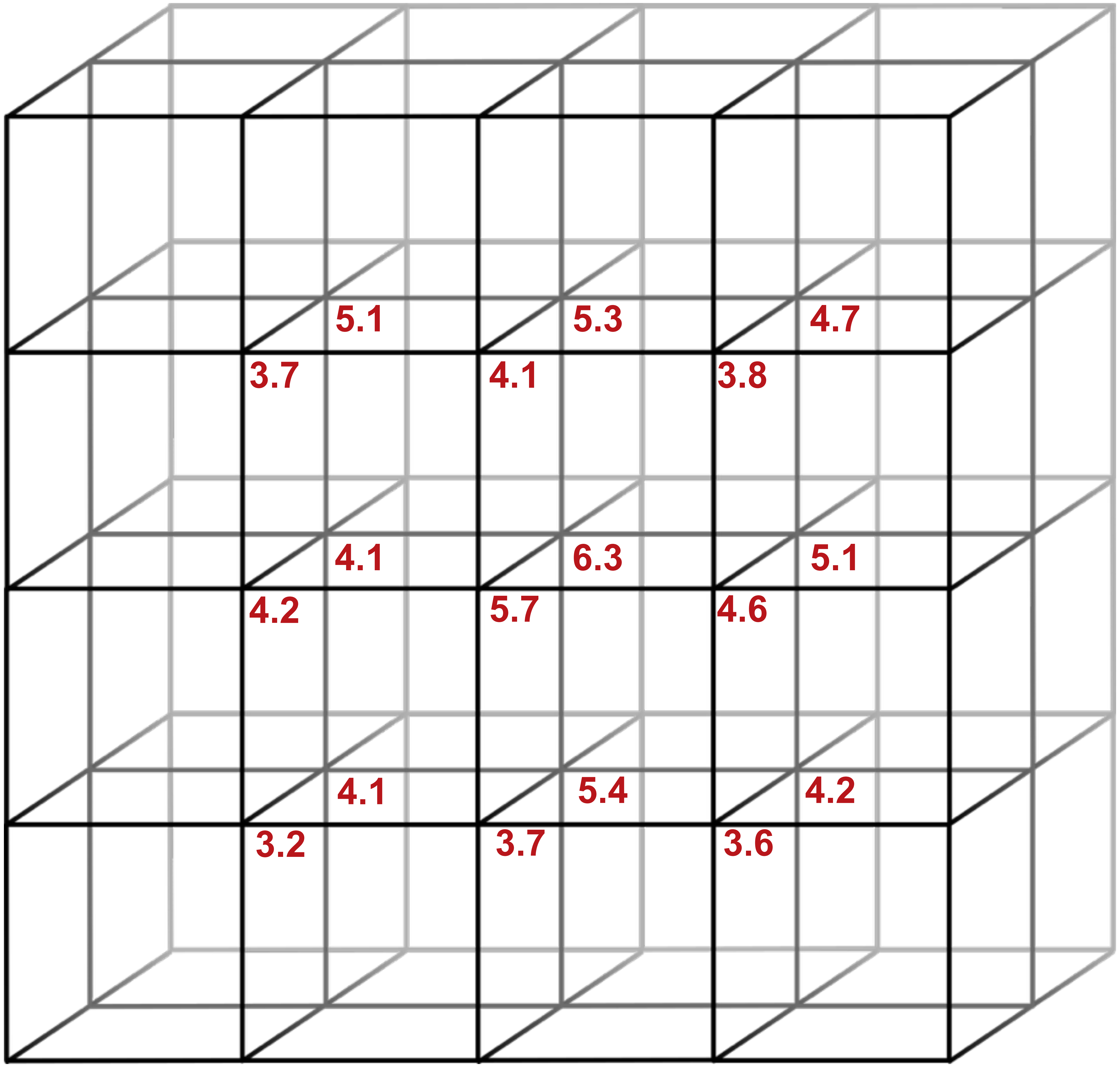
- Applied for CT, MRI, Molecular Modelling

3D-Voxel Data



3D-Voxel Data

Iso-surface at 5.0



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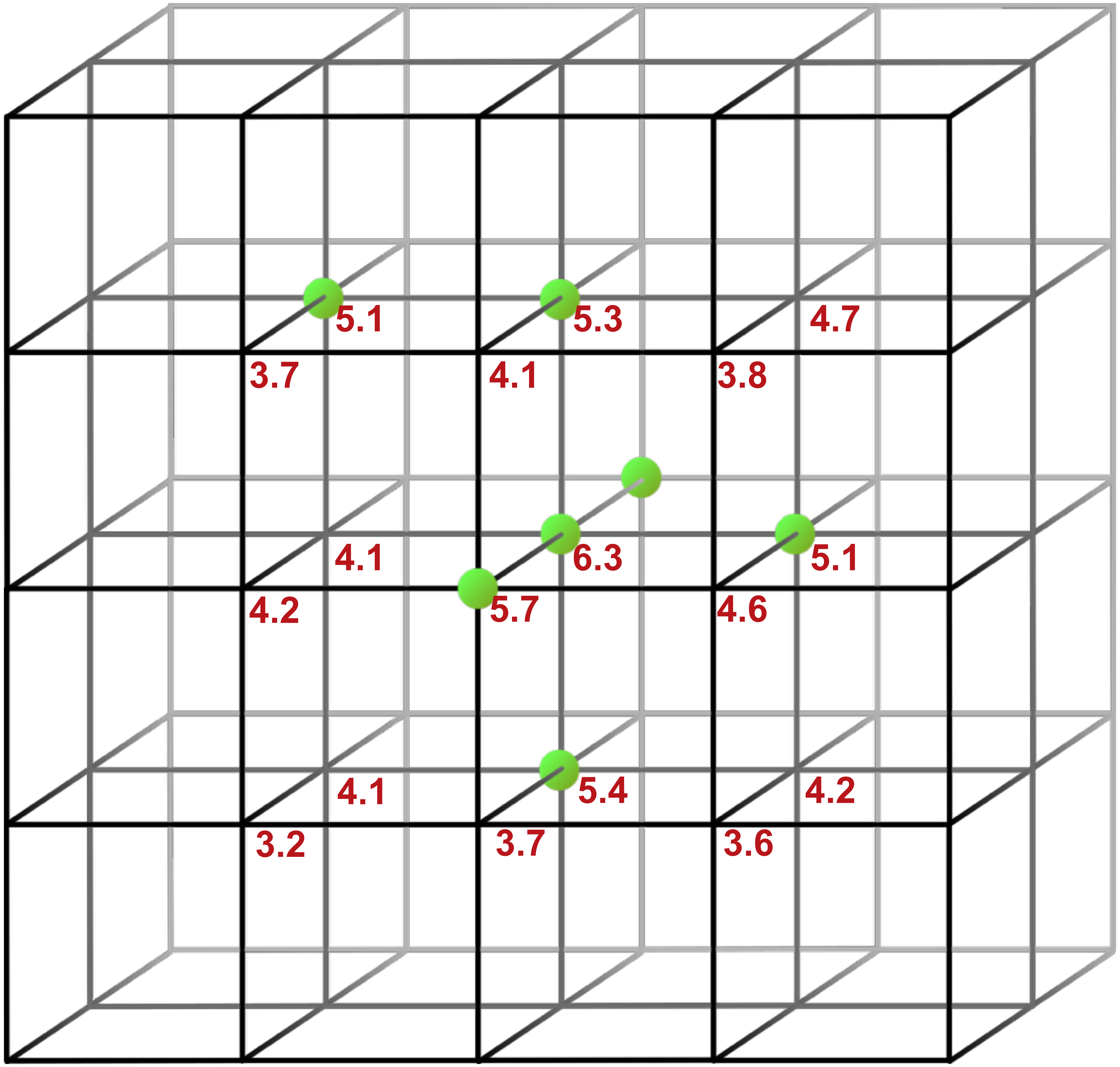

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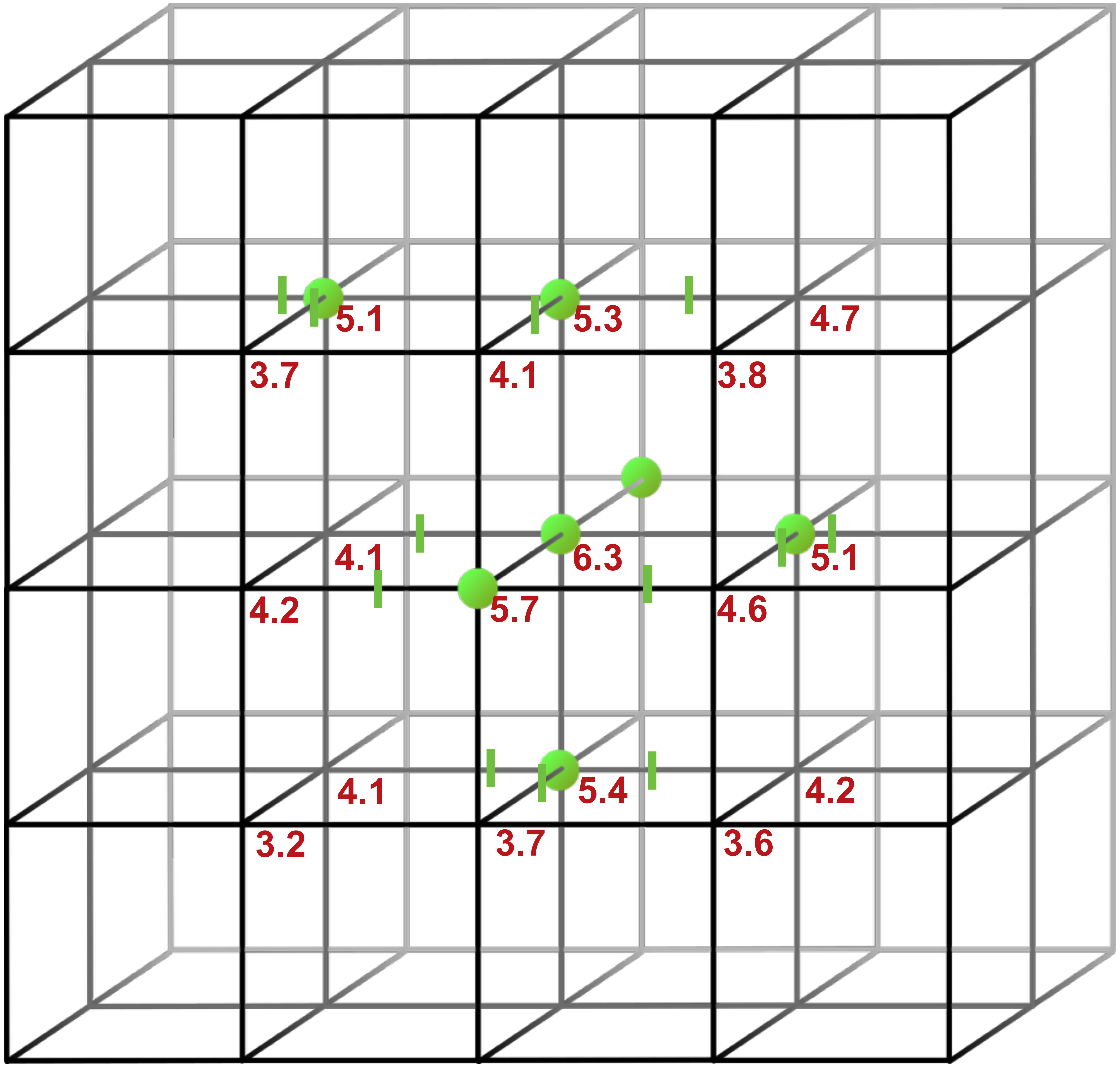
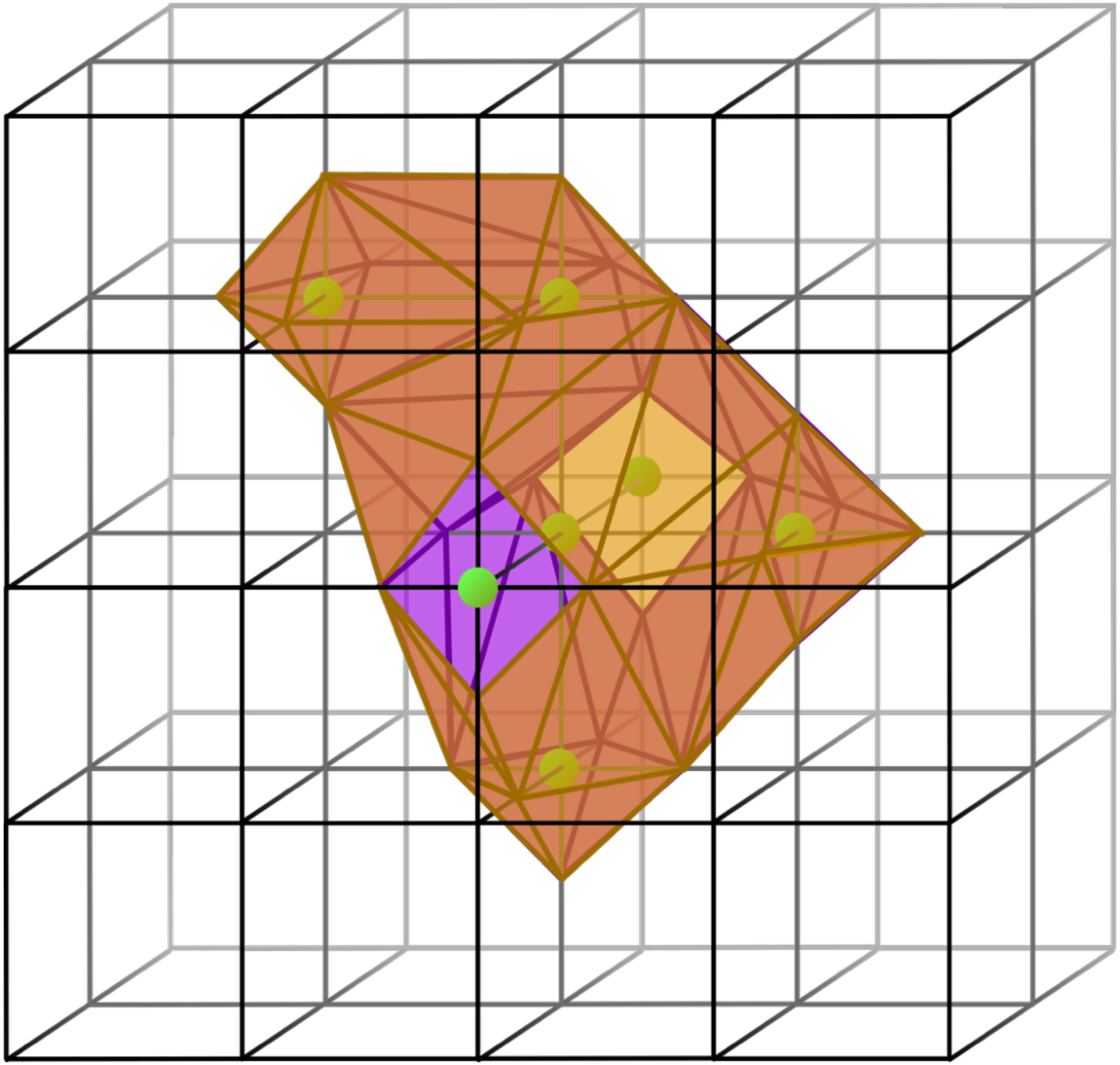
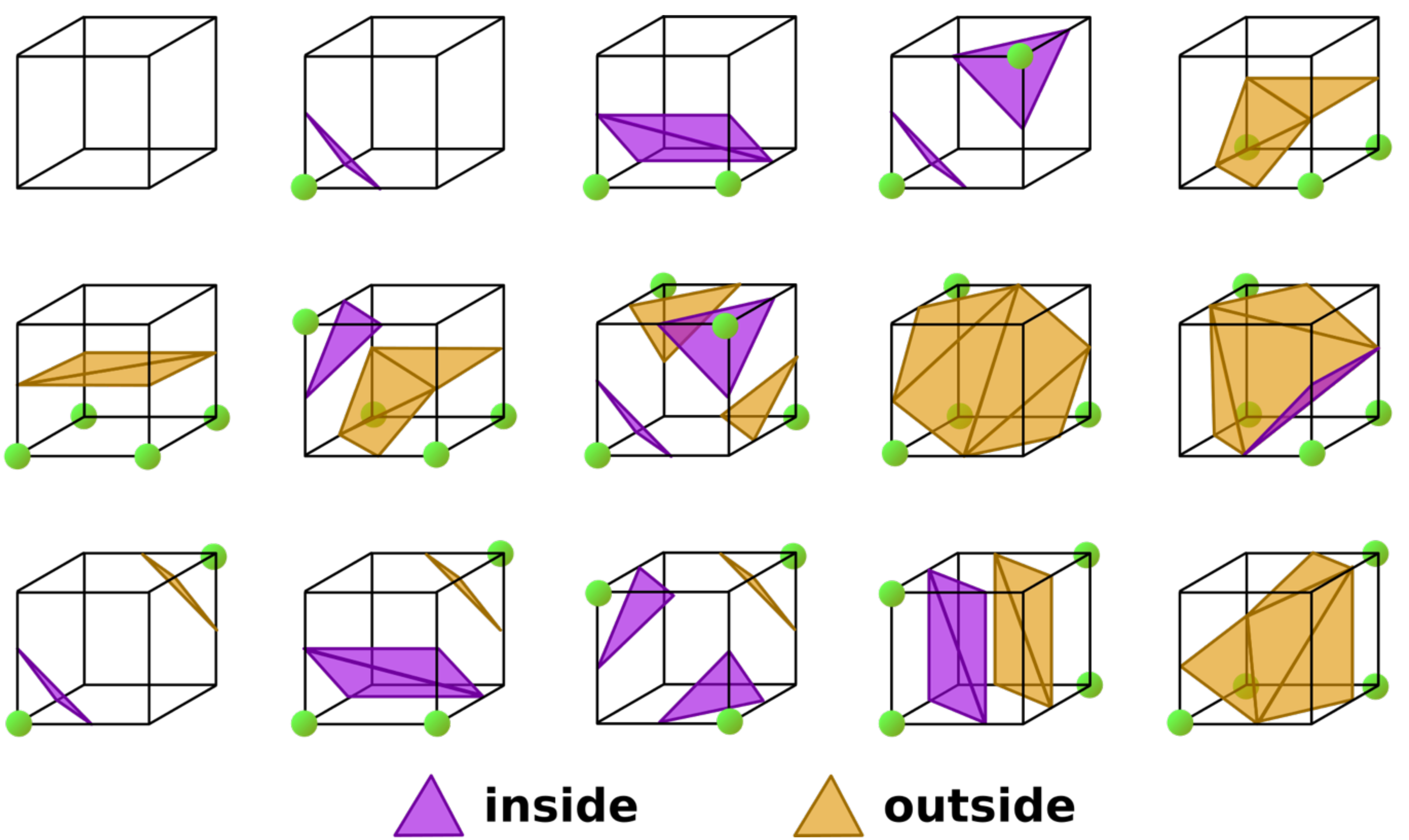


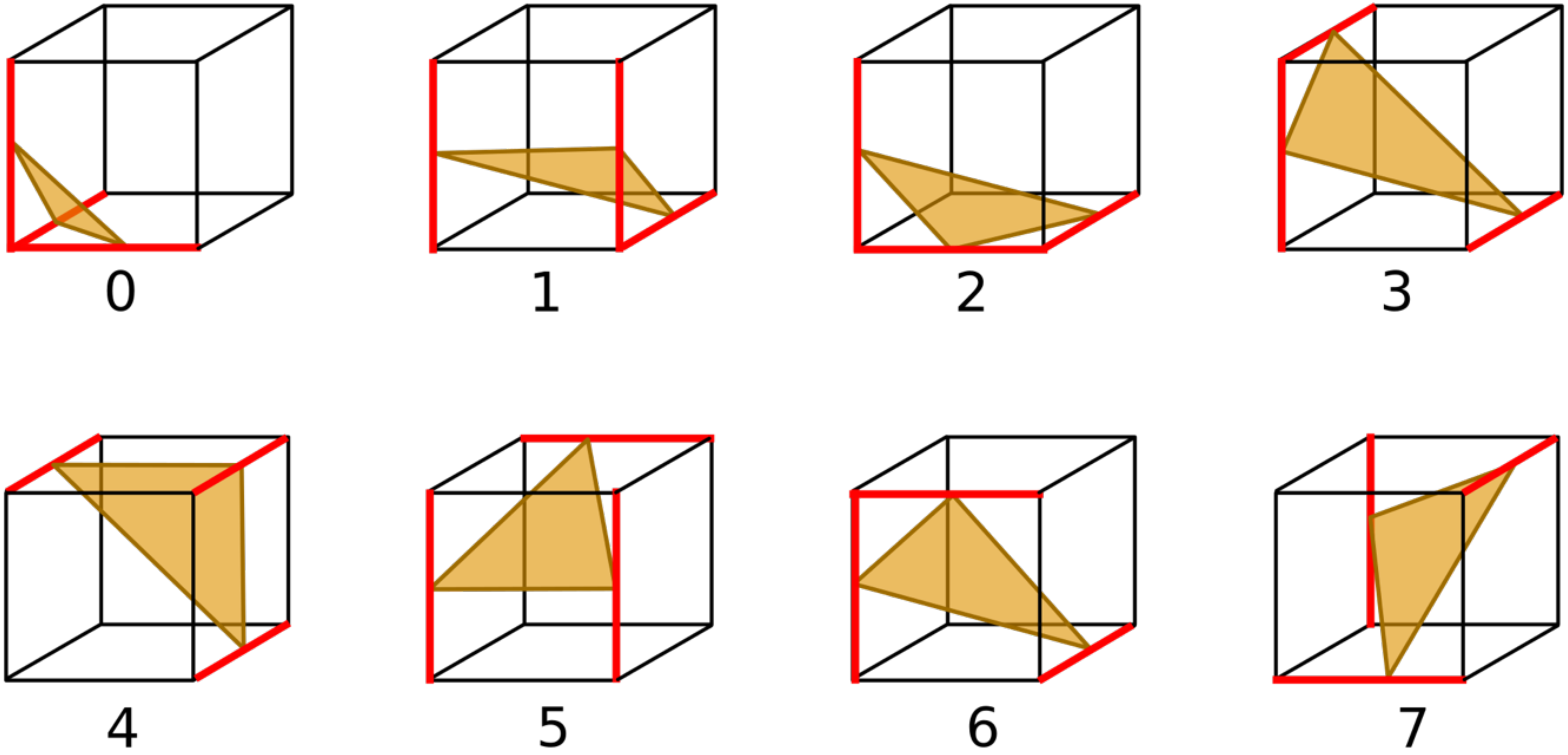
Individual Cube's Triangles Connect to Surface



256 Cubes with Triangles Derived From 15 Base (+8) Cube Families



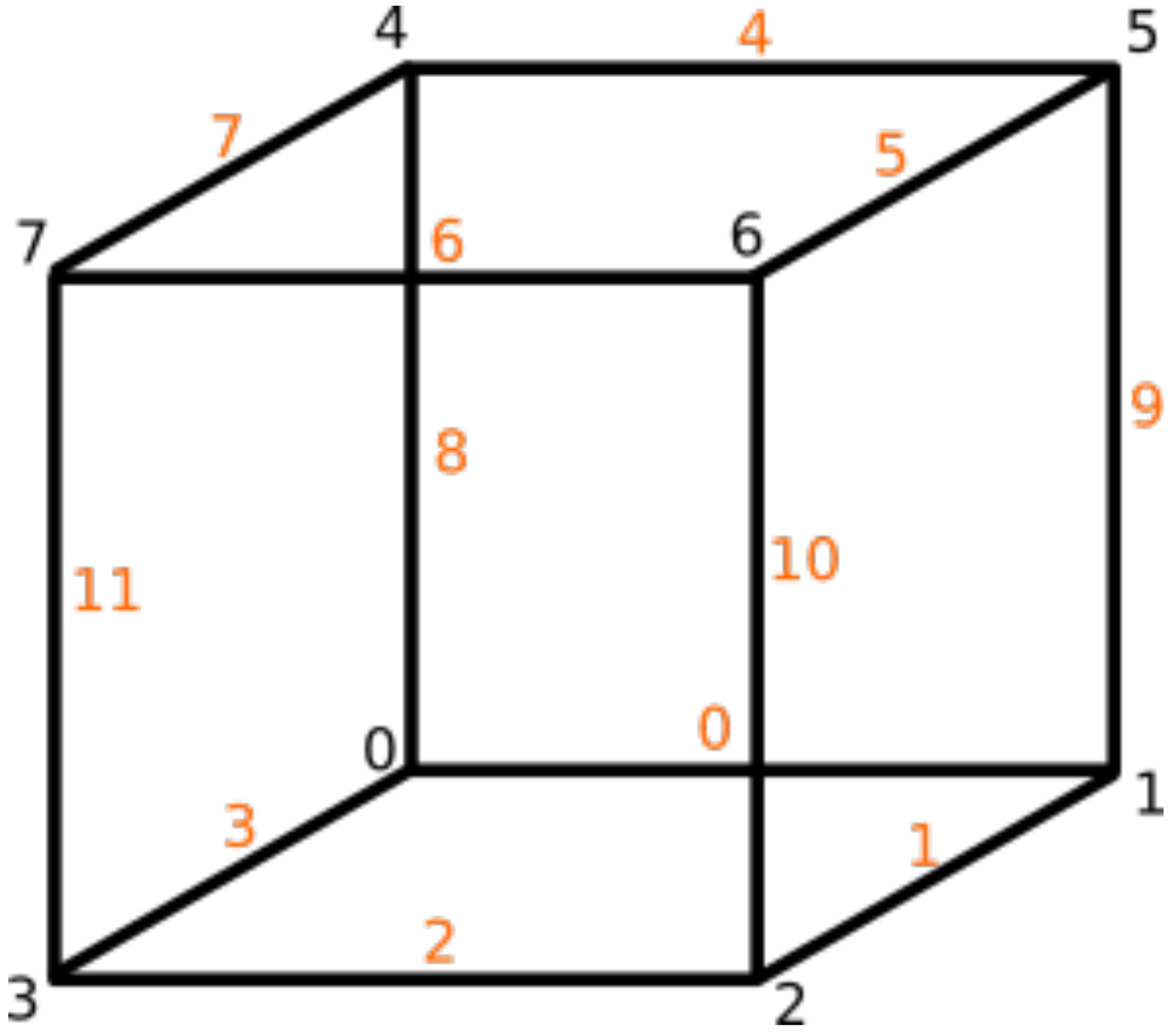
Triangles Can be Classified by 8 Edge-Groups



The Beauty: Pure Speed Through Lookup Tables

A **cube specific 8-bit key** is created from 8 corners (in or out)

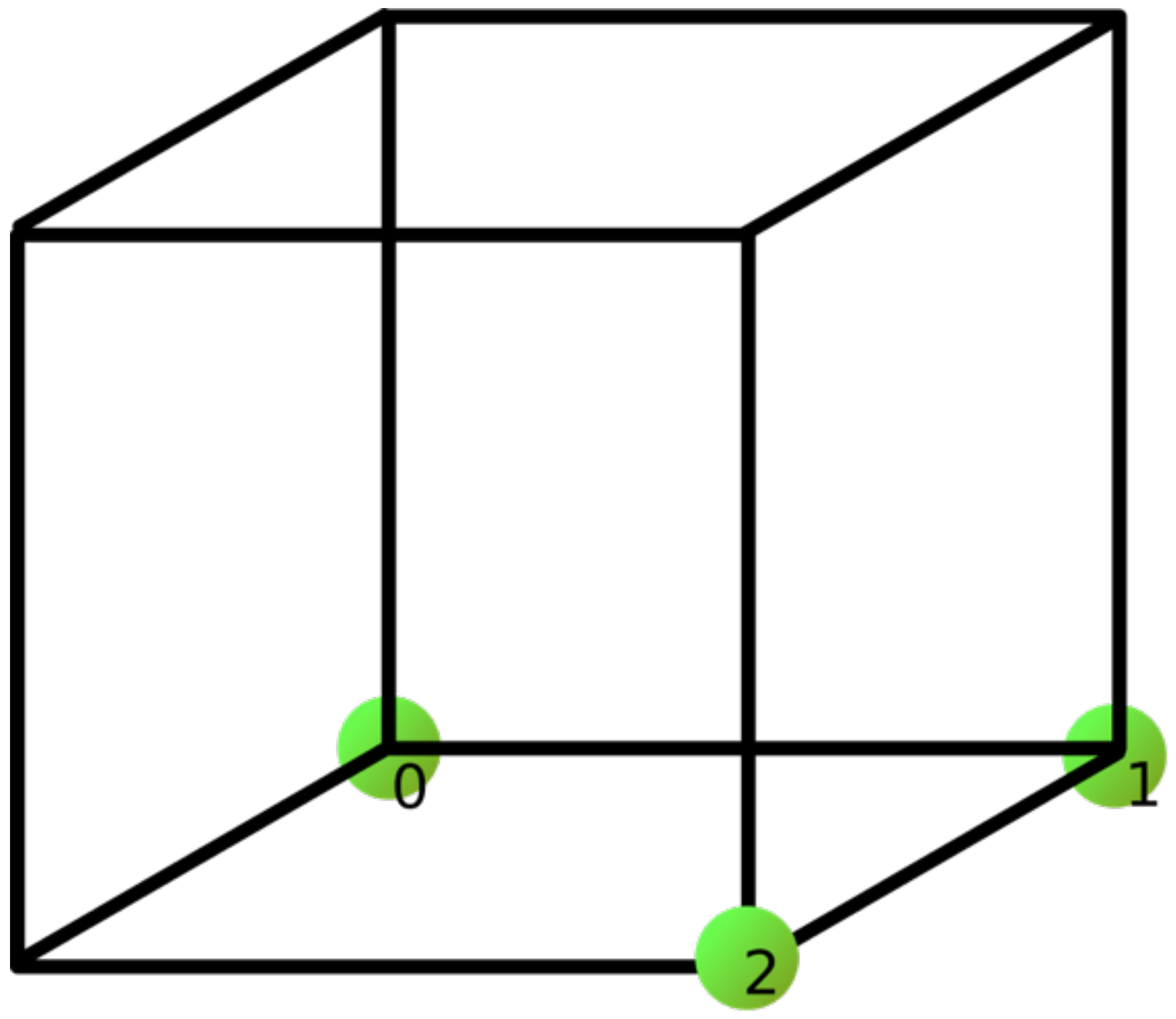
```
public static final int[] EDGE_TABLE = {
        0x000, 0x109, 0x203, 0x30a, 0x406, 0x50f, 0x605, 0x70c,
        0x80c, 0x905, 0xa0f, 0xb06, 0xc0a, 0xd03, 0xe09, 0xf00,
        0x190, 0x099, 0x393, 0x29a, 0x596, 0x49f, 0x795, 0x69c,
        0x99c, 0x895, 0xb9f, 0xa96, 0xd9a, 0xc93, 0xf99, 0xe90, … }

public static final int[][] FACE_TABLE =
        {{},
        {0, 8, 3},
        {0, 1, 9},
        {1, 8, 3, 9, 8, 1},
        {1, 2, 10},
        {0, 8, 3, 1, 2, 10},
        {9, 2, 10, 0, 2, 9},
        {2, 8, 3, 2, 10, 8, 10, 9, 8},
        {3, 11, 2}, … }
```



The Triangulation Process

For all cubes do

- build key from 8 corners (00000111b = 7)
- lookup affected edges: 0x70c
- calculate vertexes on affected edges
- lookup faces: {2, 8, 3, 2, 10, 8, 10, 9, 8}
- create triangles connecting vertexes



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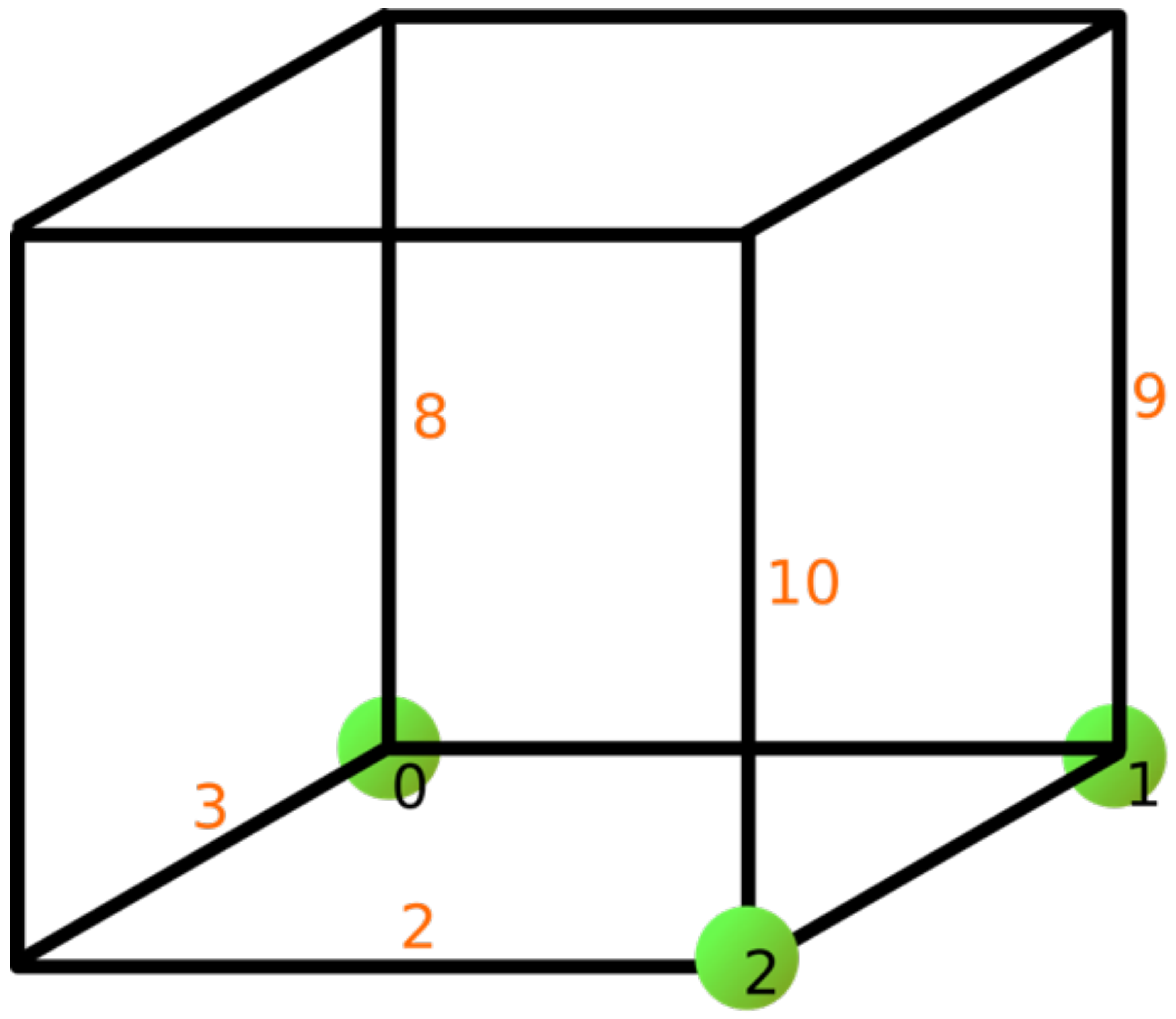

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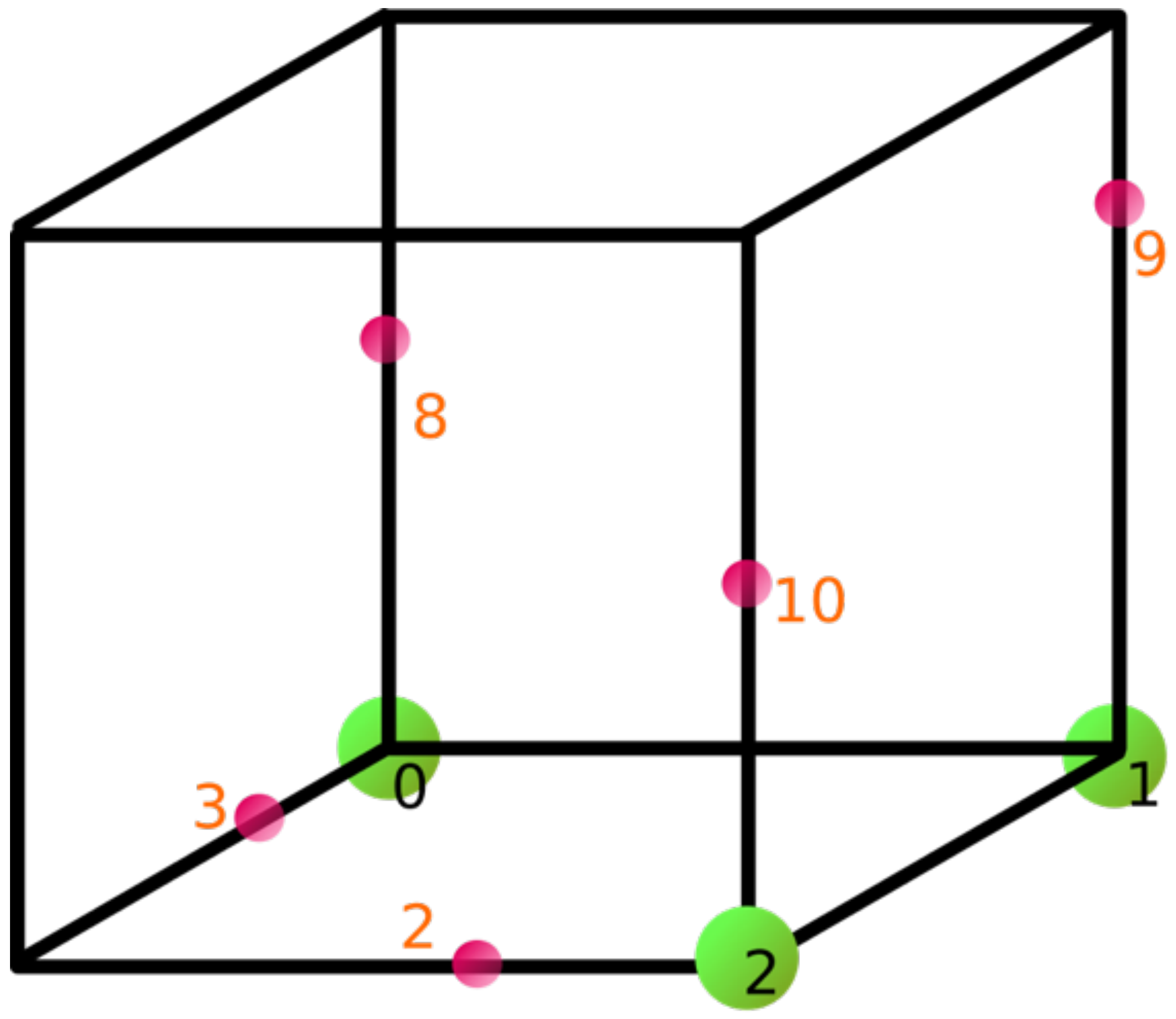

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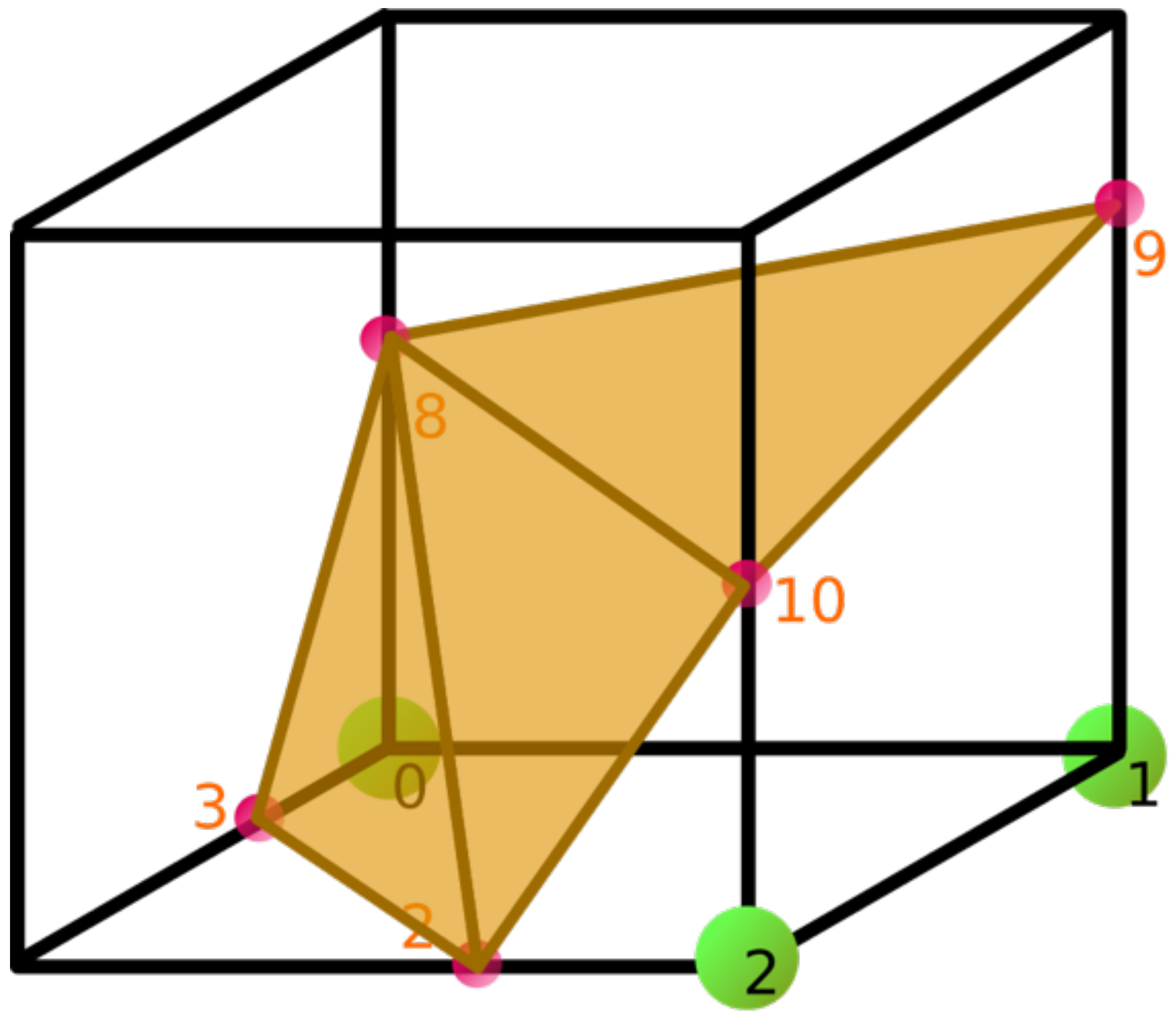
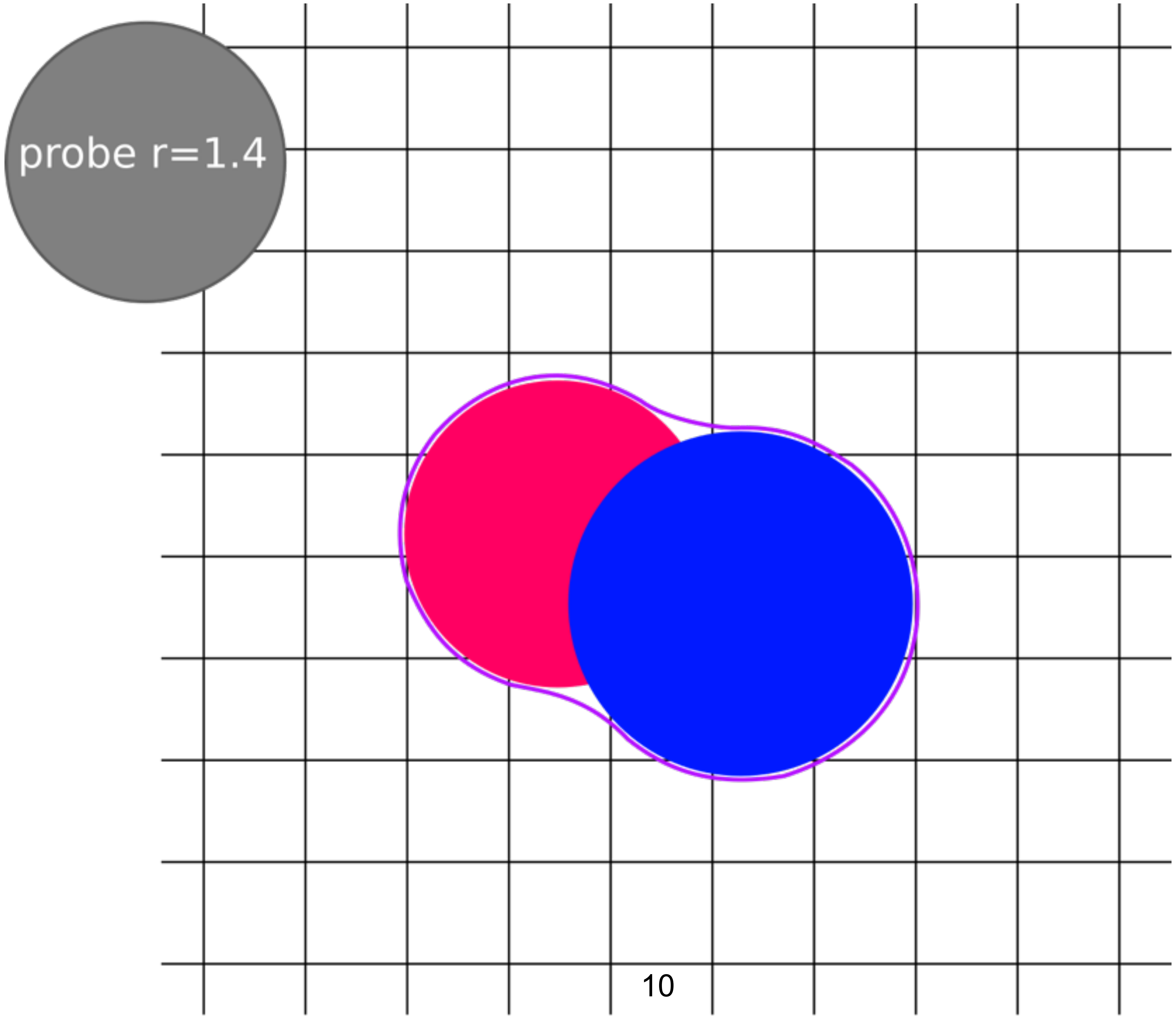


How Does this help to create a Connolly surface?
Create Voxel Grid

For every atom
   set close grid points to VDW-radius - distance



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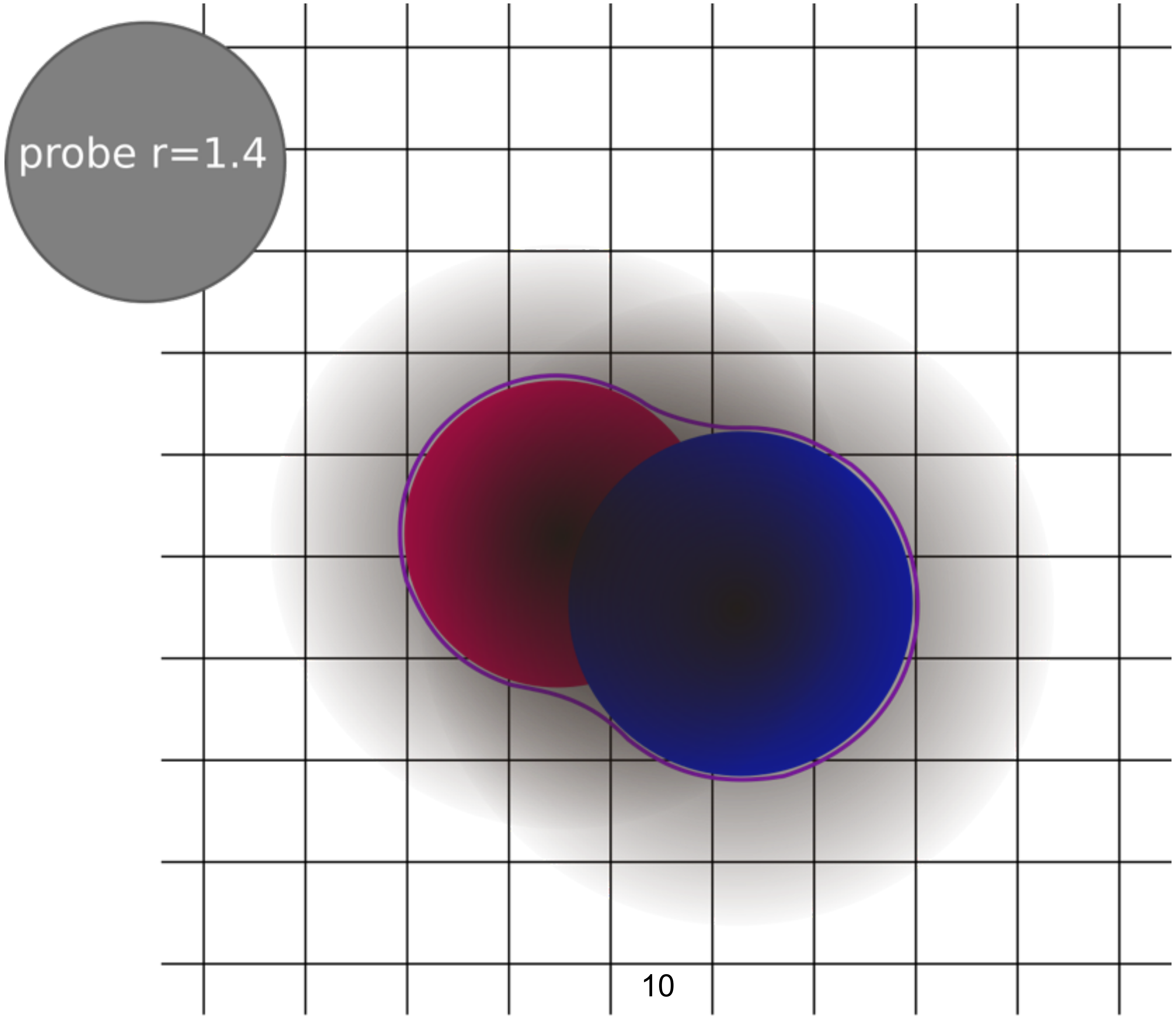
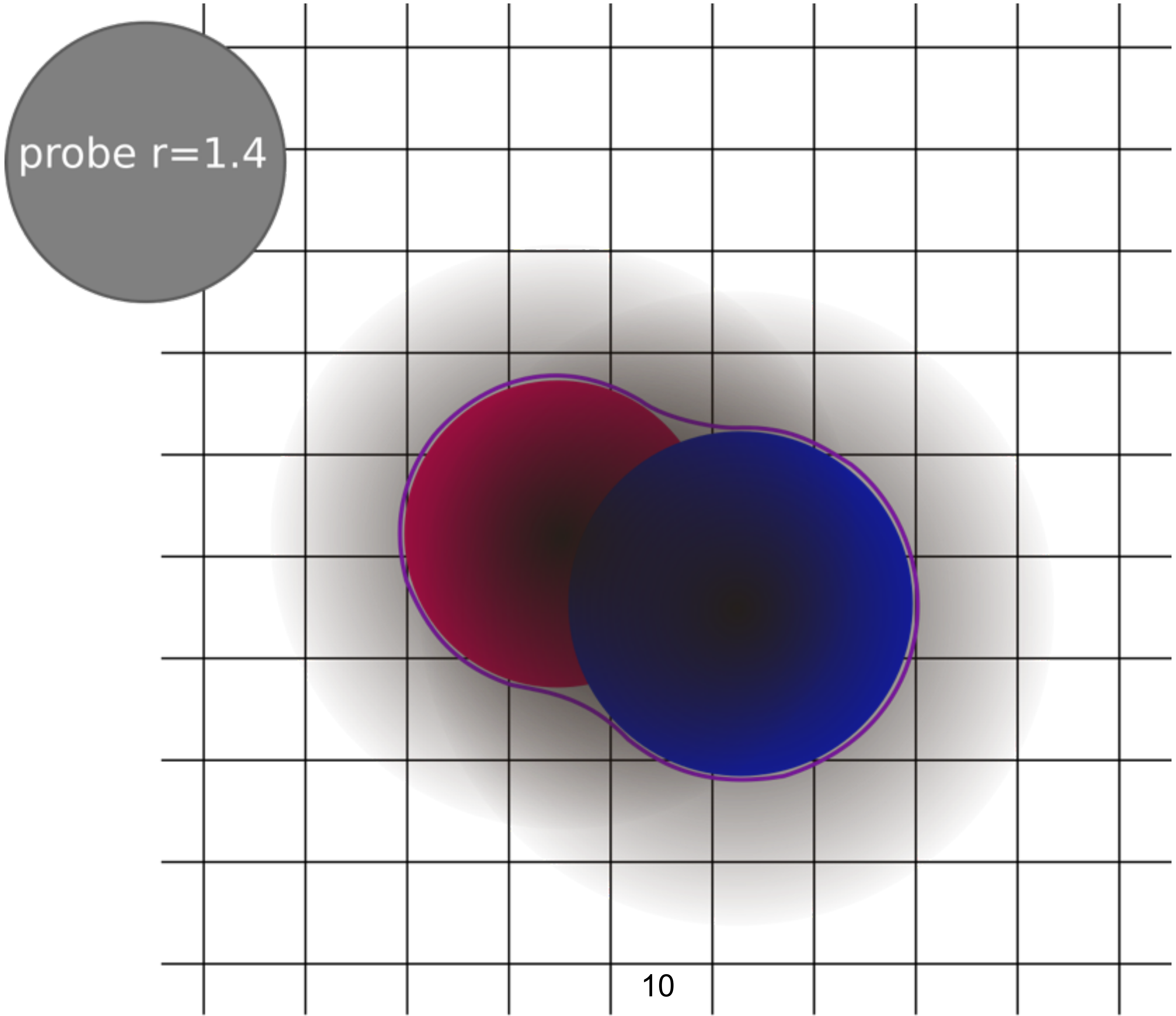


How Does this help to create a Connolly surface?
Create Voxel Grid

```
For every grid edge with separating positive from negative volume
    determine edge position p1 with value=0
    for every grid point p2 within probe radius
        set value to min(value, distance - probeRadius)
```



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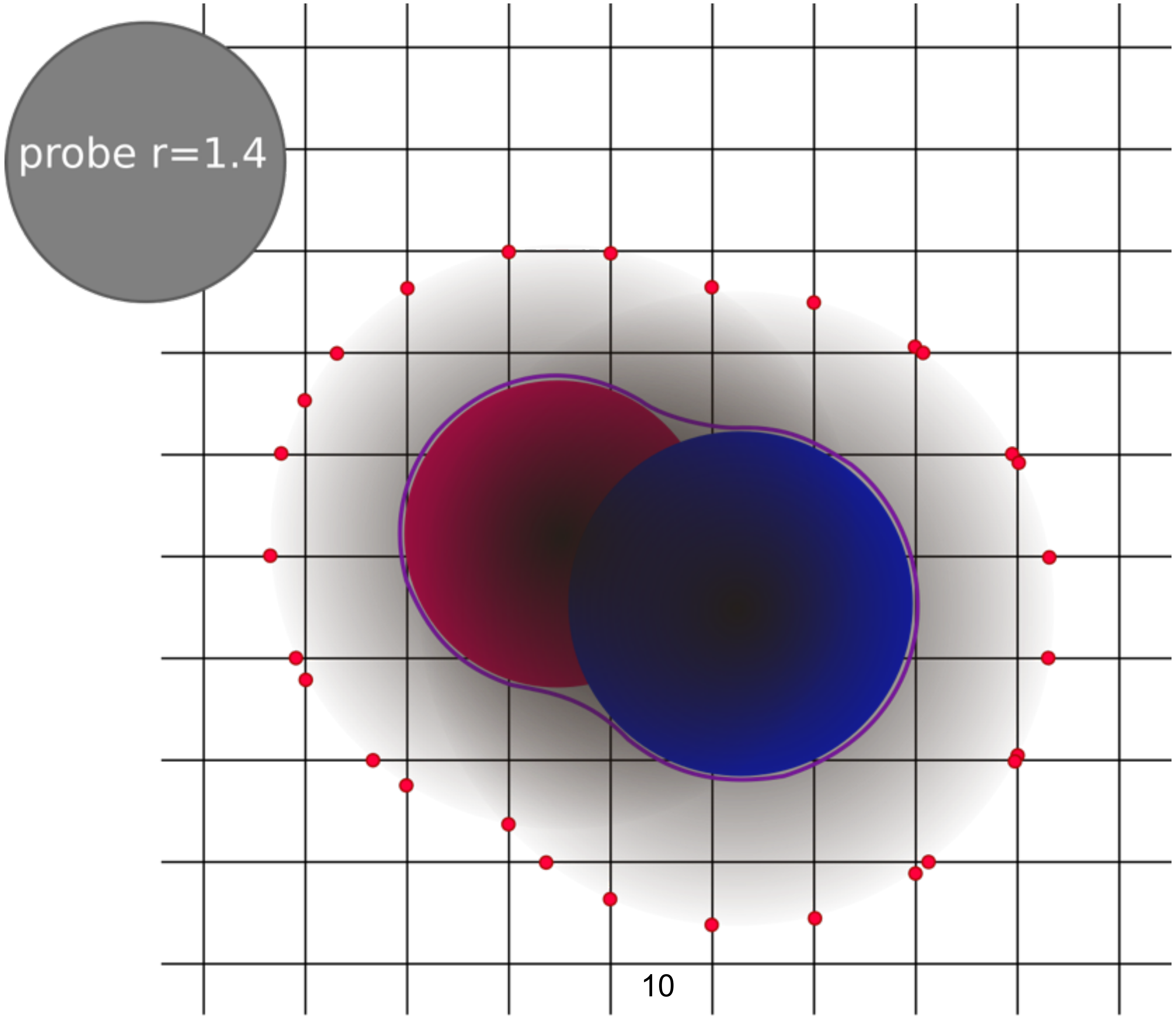

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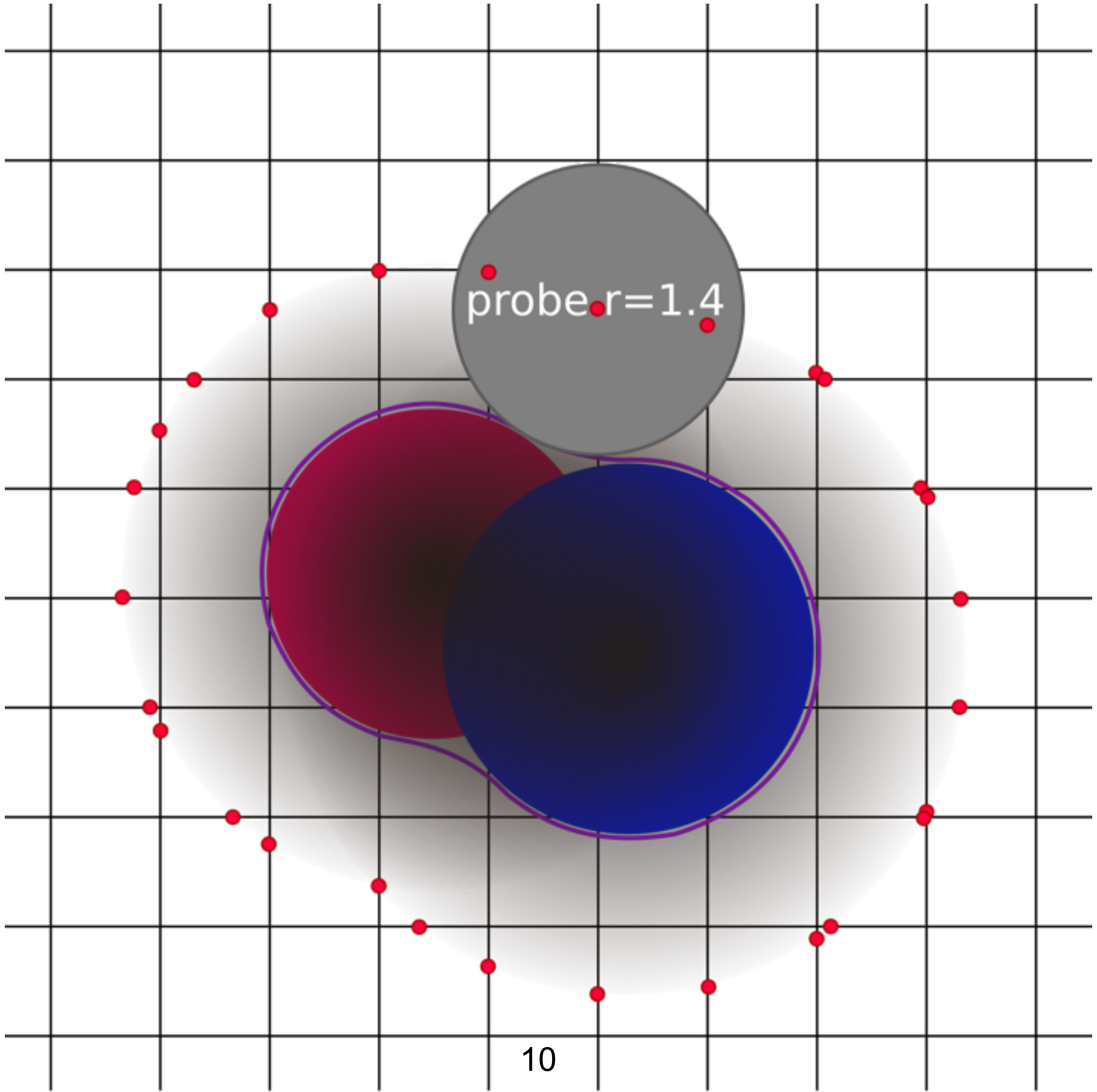

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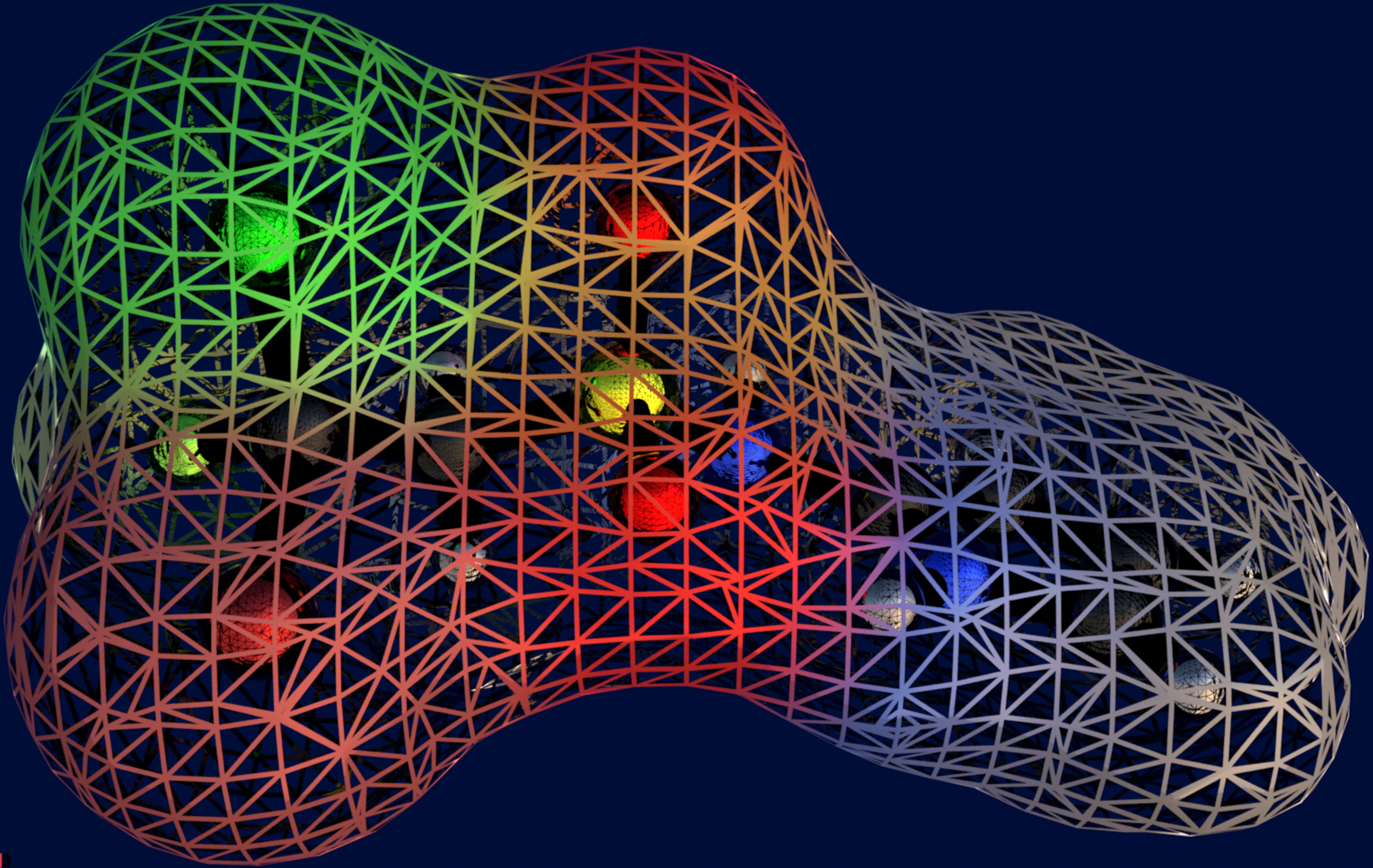
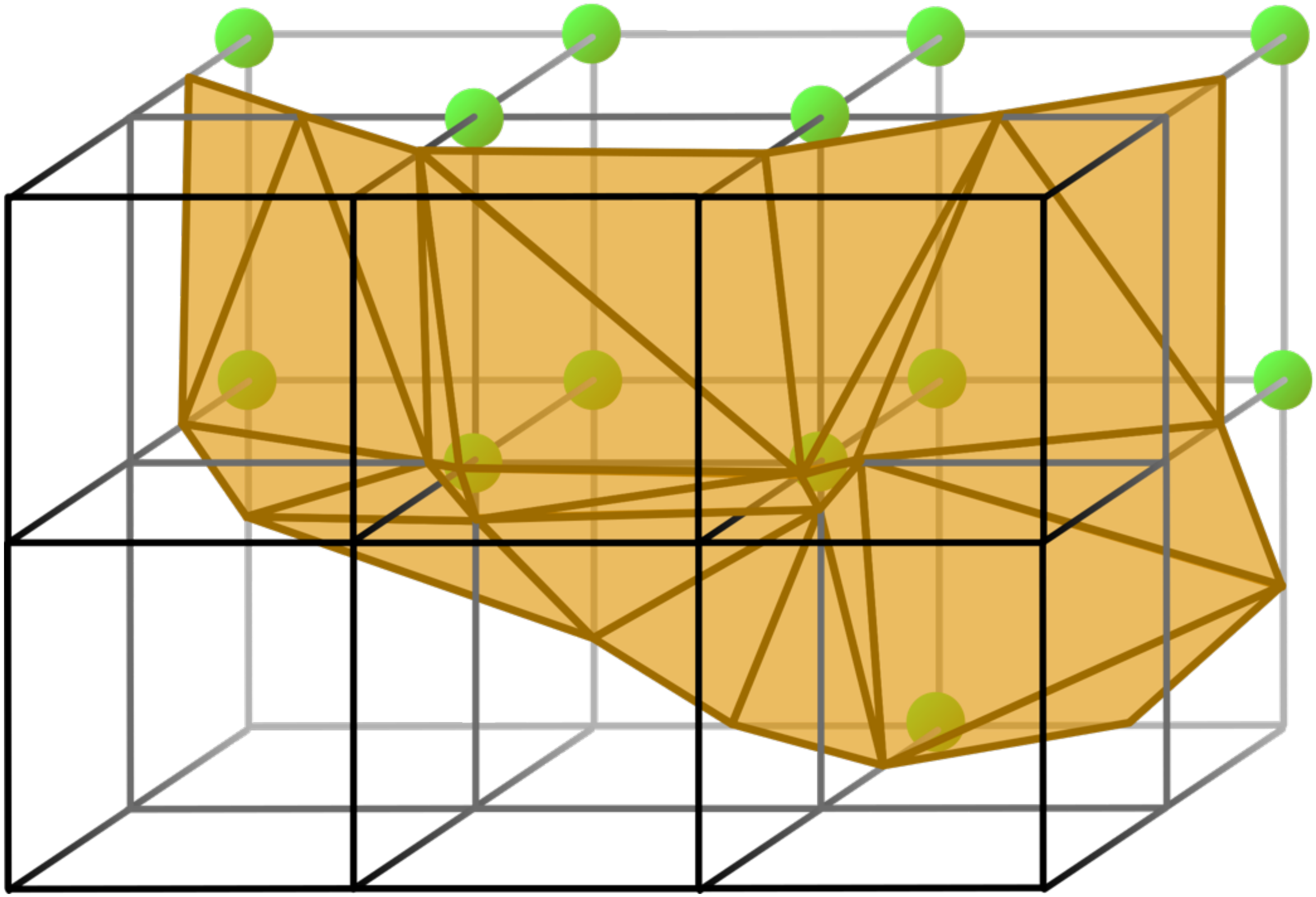
inspired by Tom Goddard,
“Molecular Surface Algorithm”,
Oct 14, 2013,
www.cgl.ucsf.edu/chimera/data/surface-oct2013/surface.html

Problem: Small and skinny triangles



Avoiding Small-Area-Triangles



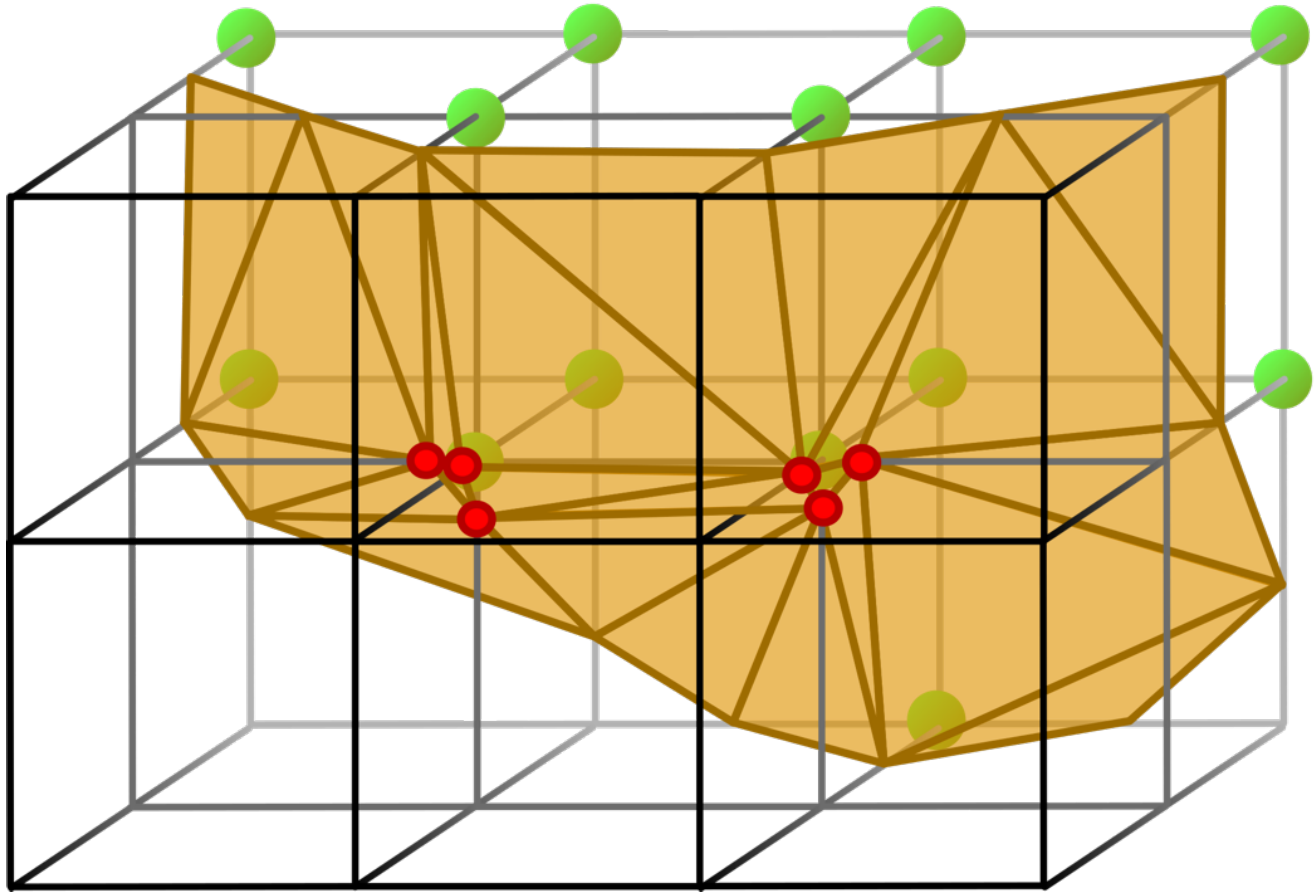
New simple procedure:

For every corner:

  if more than 1 close edge cuts

- join these edge cut positions
- remove all triangles with merged corners

Avoiding Small-Area-Triangles



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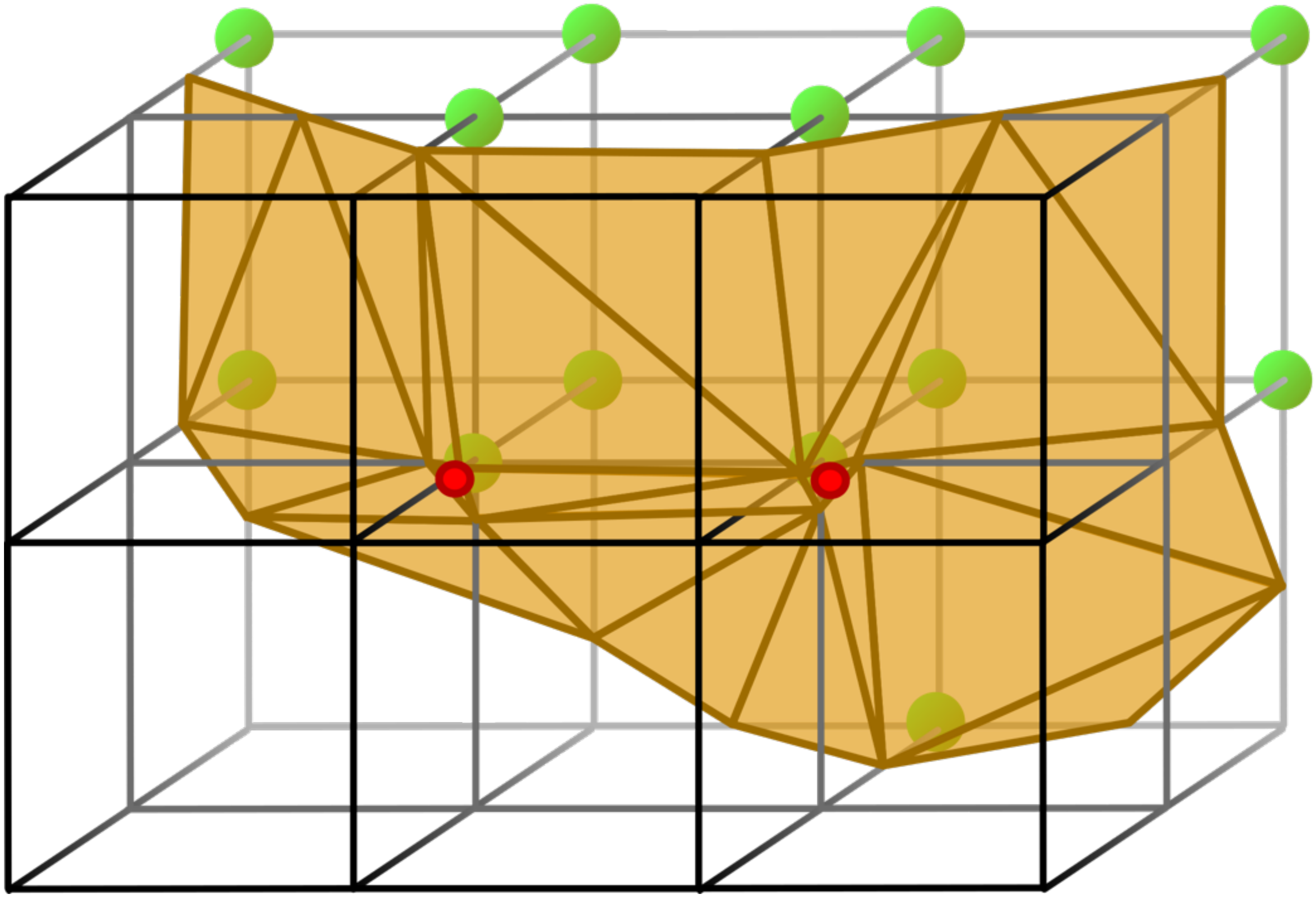

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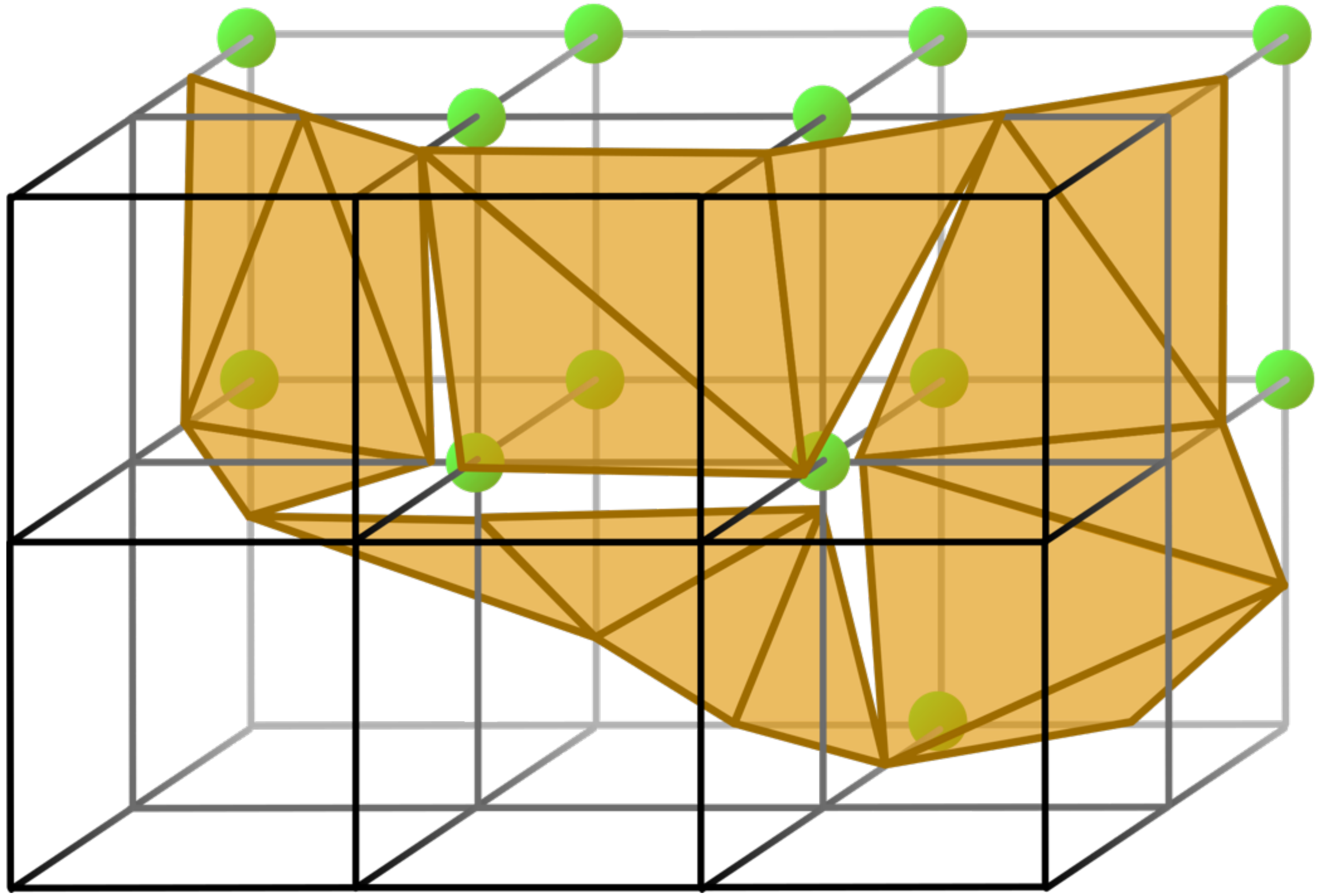

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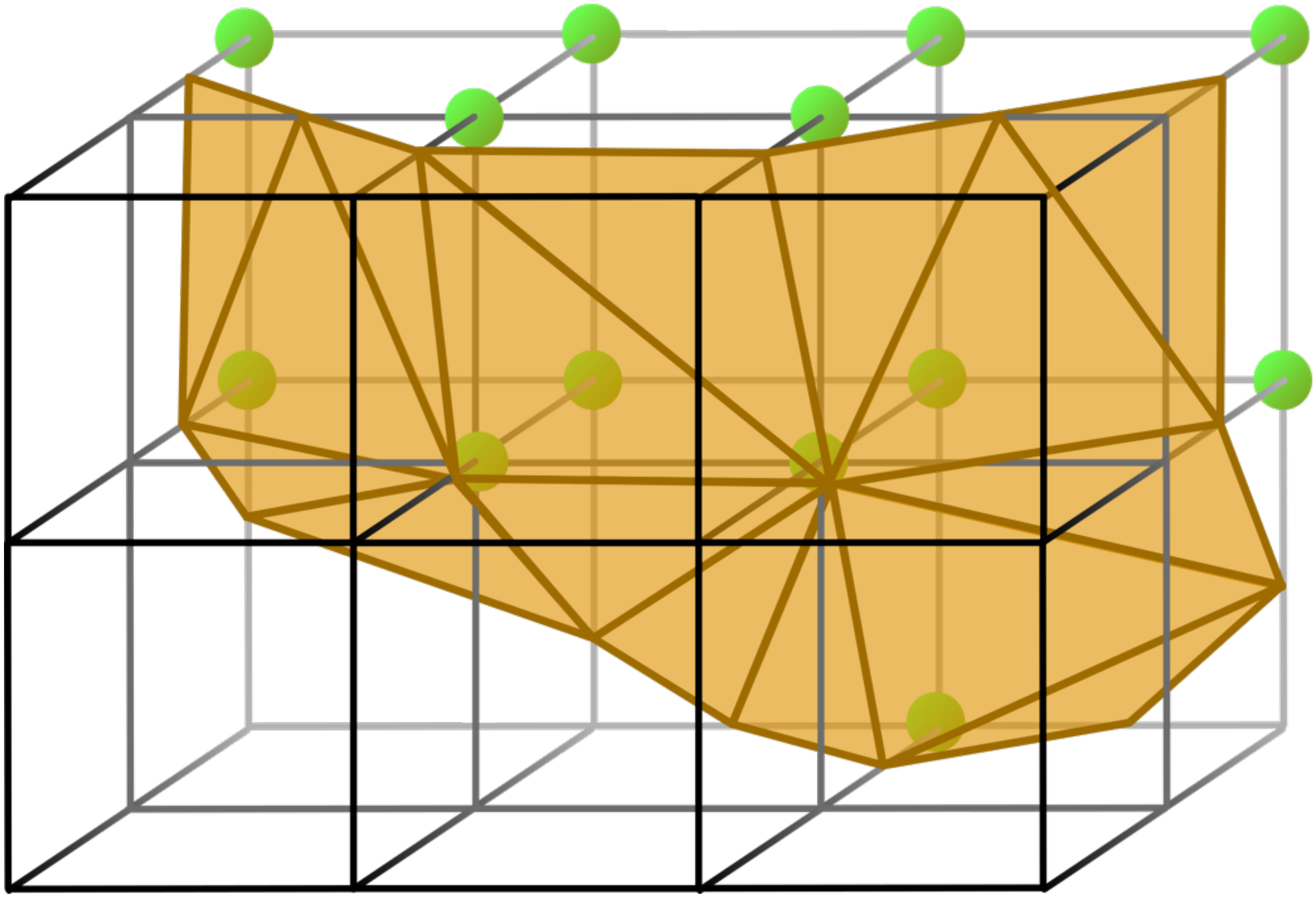

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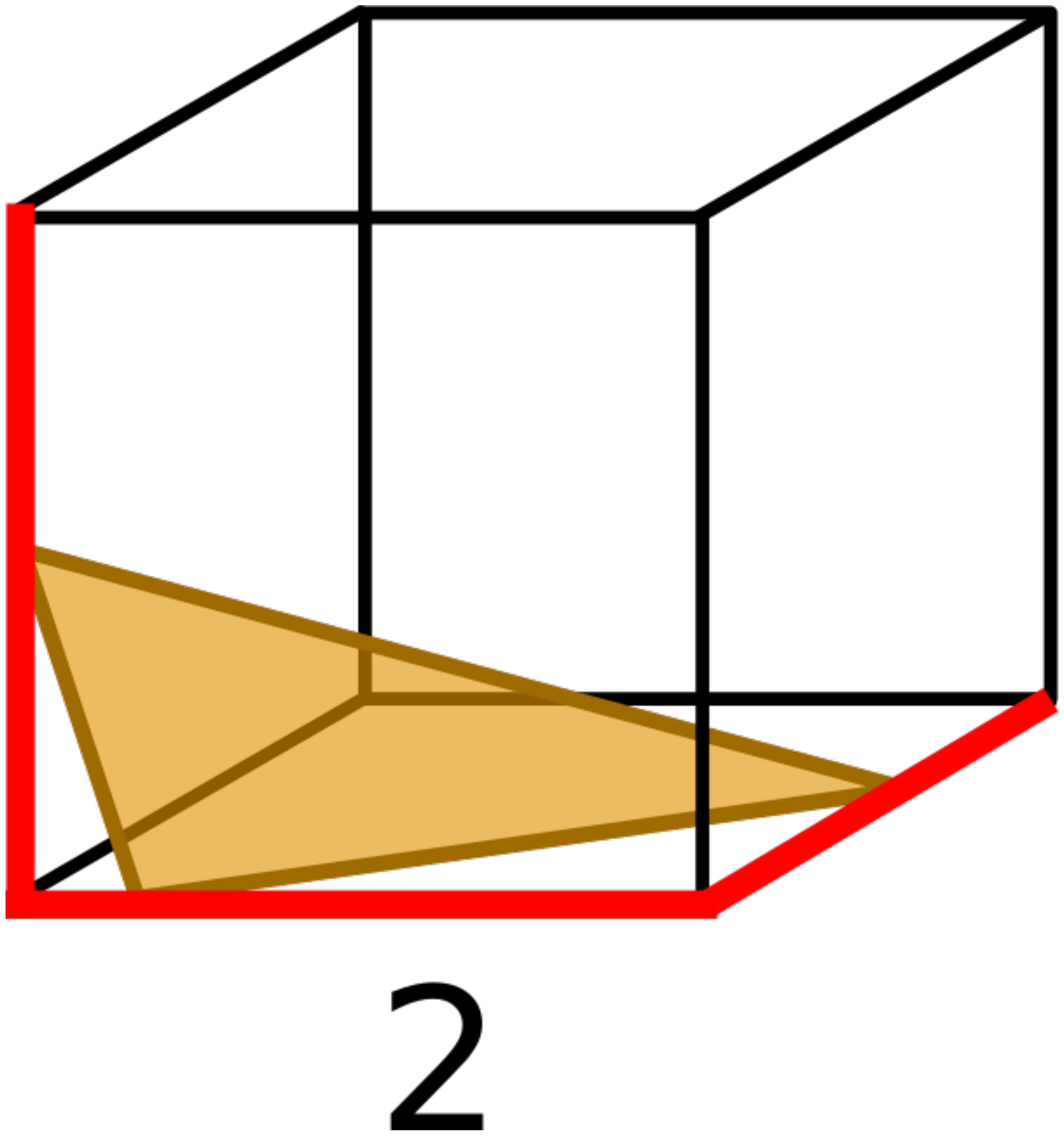
Second Source for Skinny Triangles: Edge Group 2



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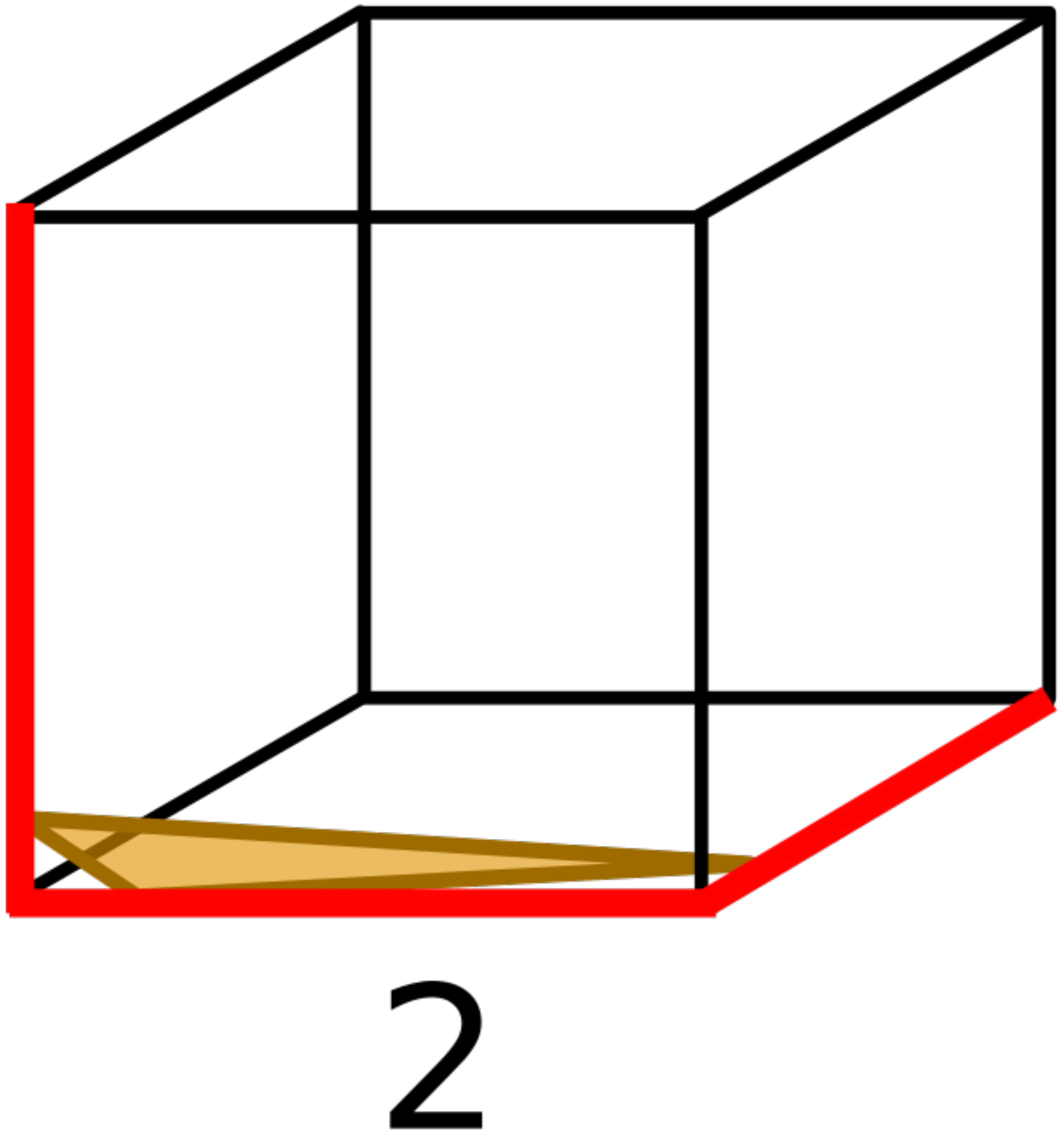

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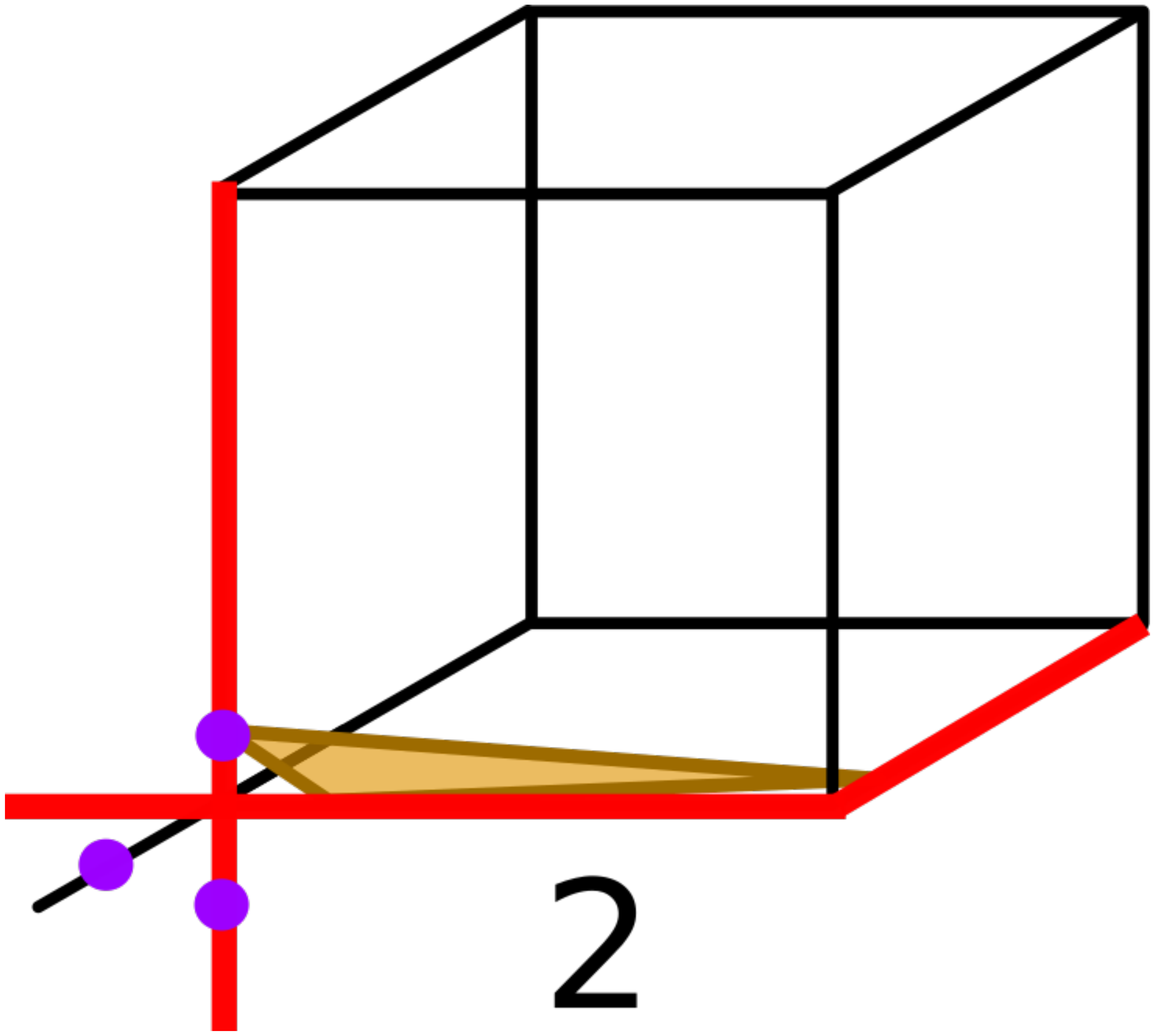

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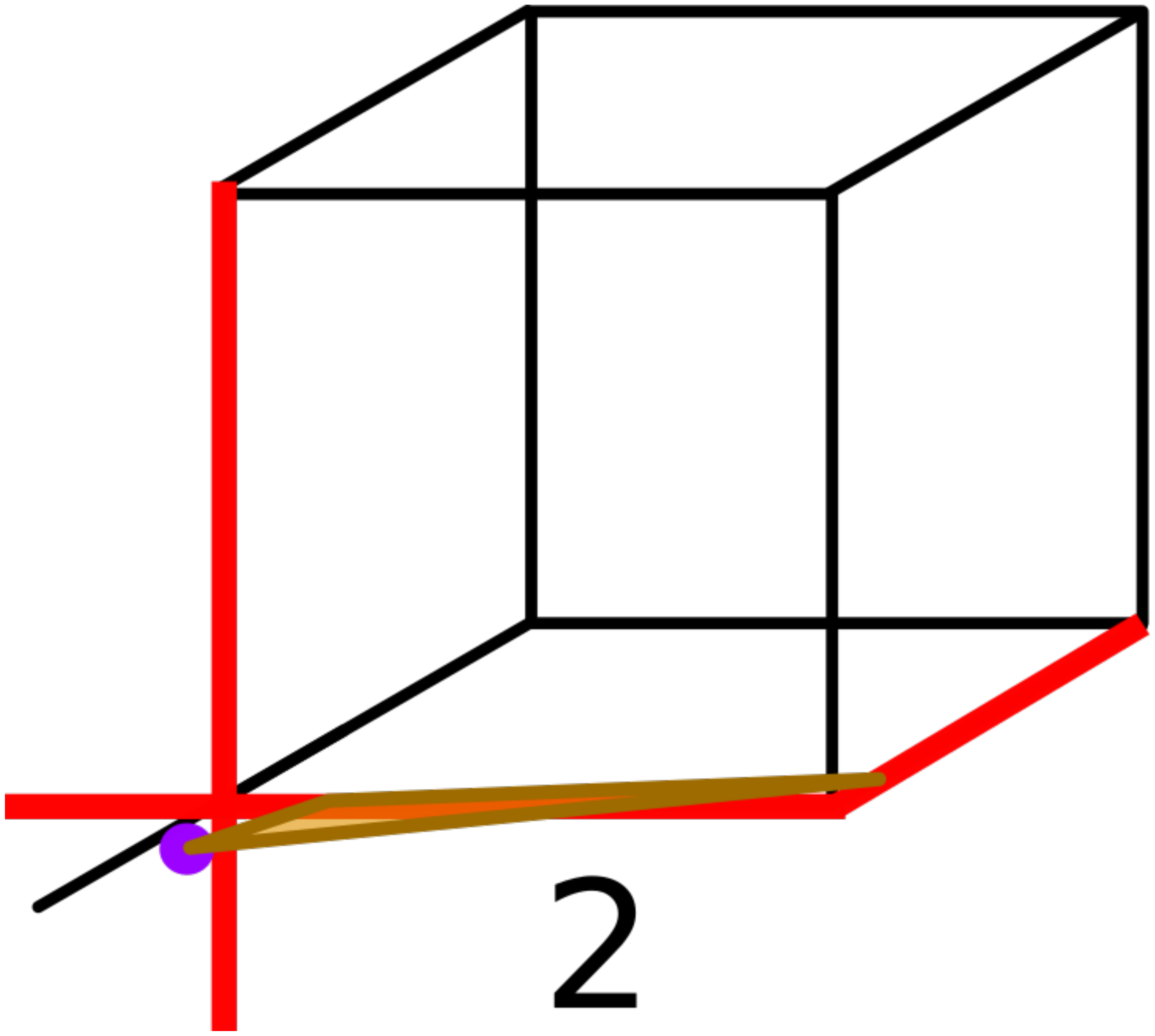
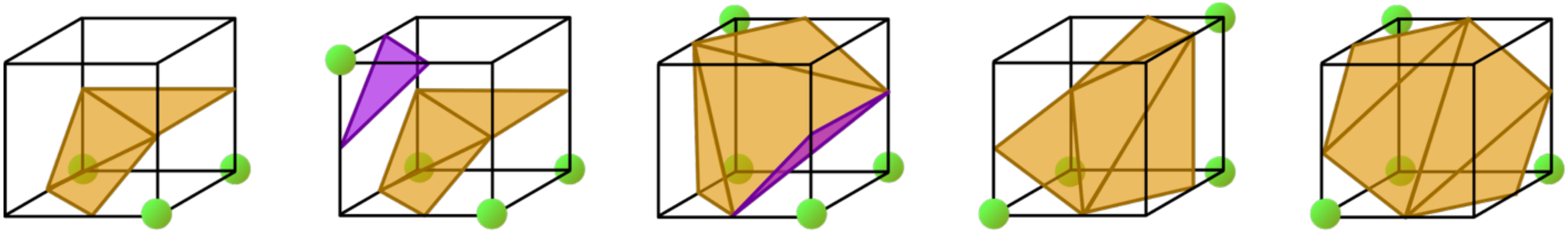


How To Avoid Edge Group 2



C. A. Dietrich, C. E. Scheidegger, J. L. D. Comba, L. P. Bedel, C. T. Silva, Comput. Sci. Eng. 11, 82 (2009)

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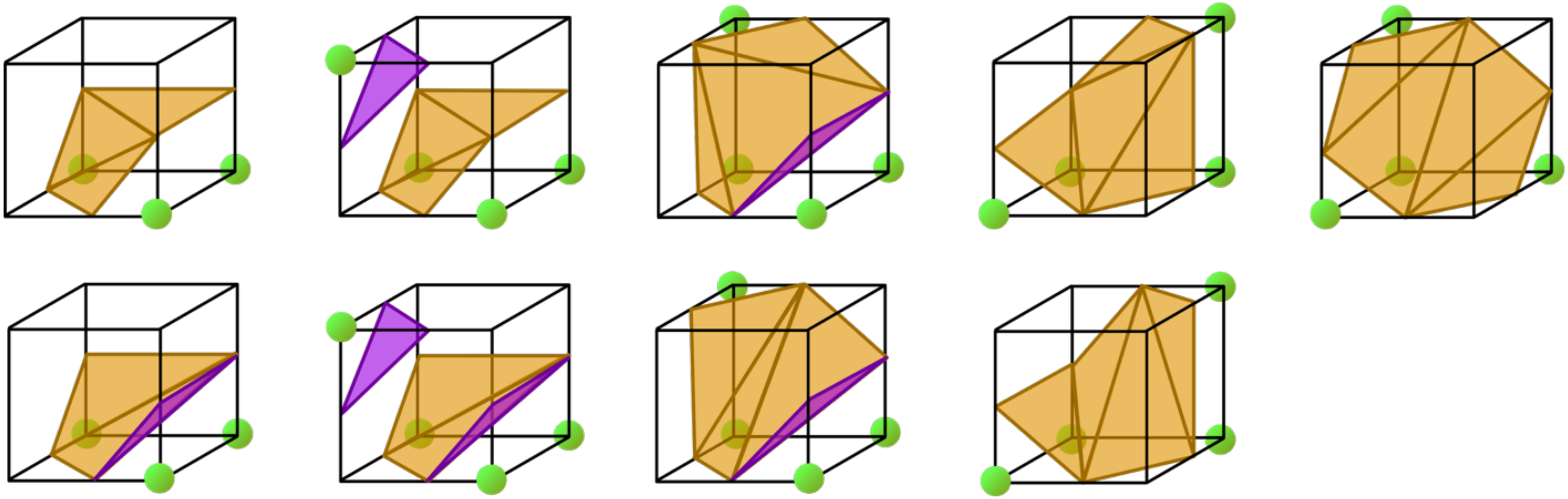

Most cubes can be triangulated in a different way to avoid edge group 2

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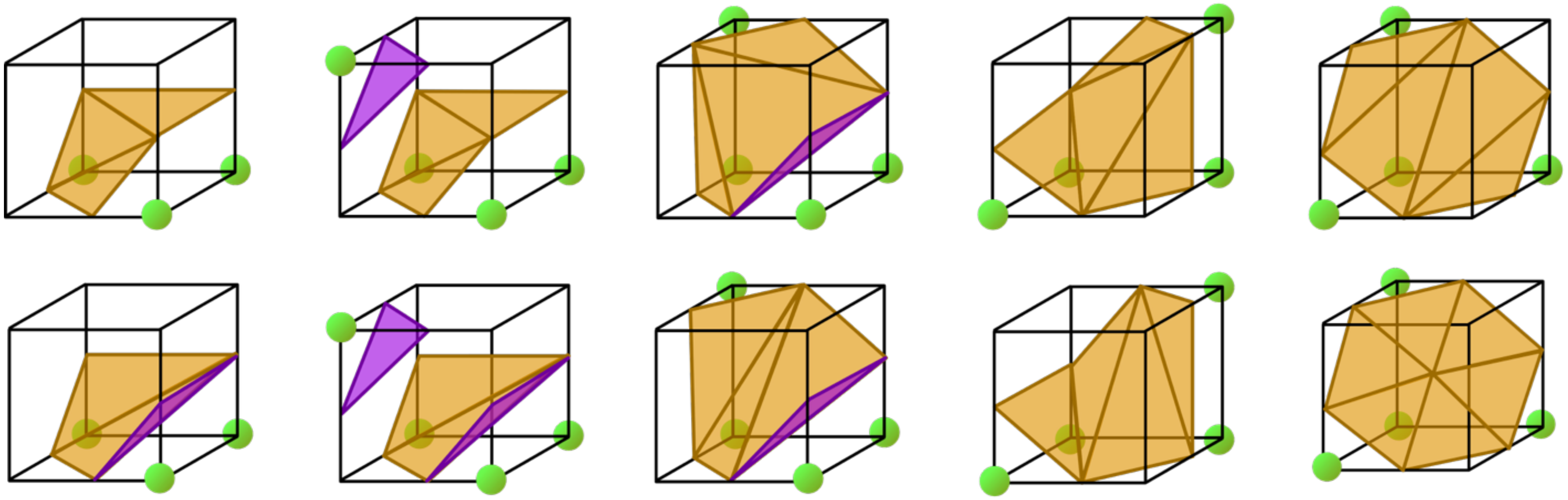
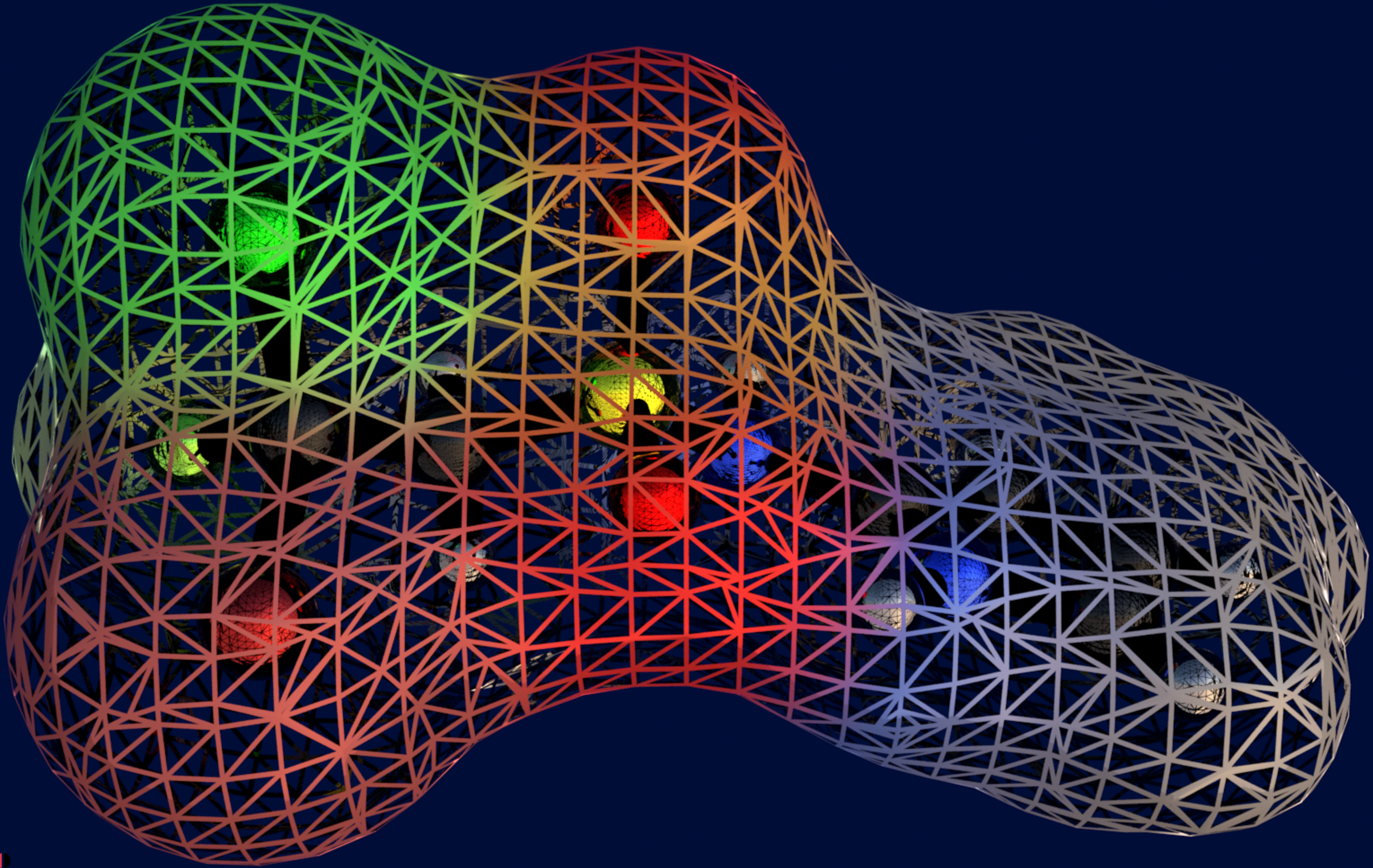


Most cubes can be triangulated in a different way to avoid edge group 2

Where triangulation without edge group 2 is impossible, we add a new vertex

C. A. Dietrich, C. E. Scheidegger, J. L. D. Comba, L. P. Bedel, C. T. Silva, Comput. Sci. Eng. 11, 82 (2009)

Original Marching Cubes: 3864 triangles, 1934 vertexes



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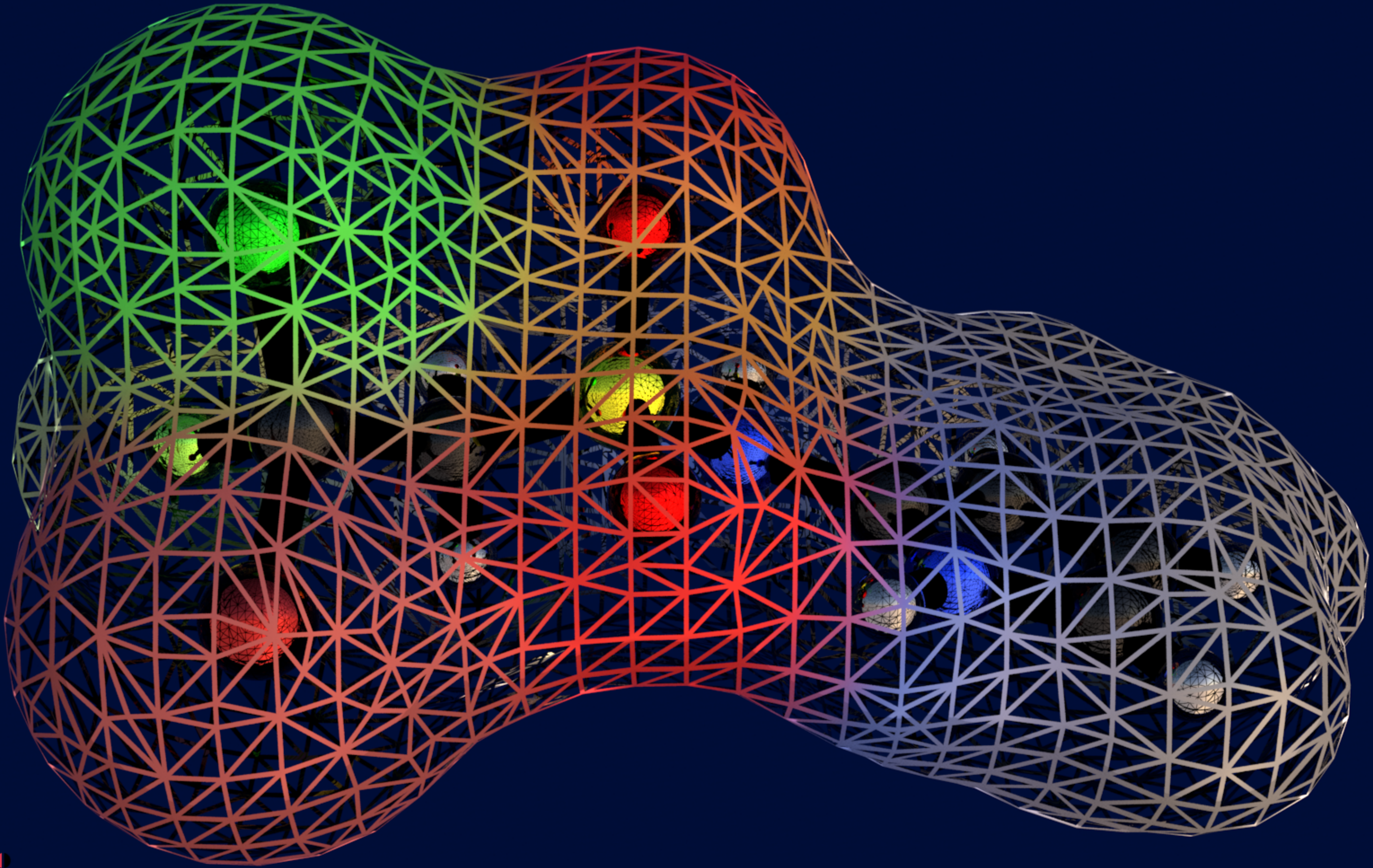
Smooth Marching Cubes: 2956 triangles, 1480 vertexes



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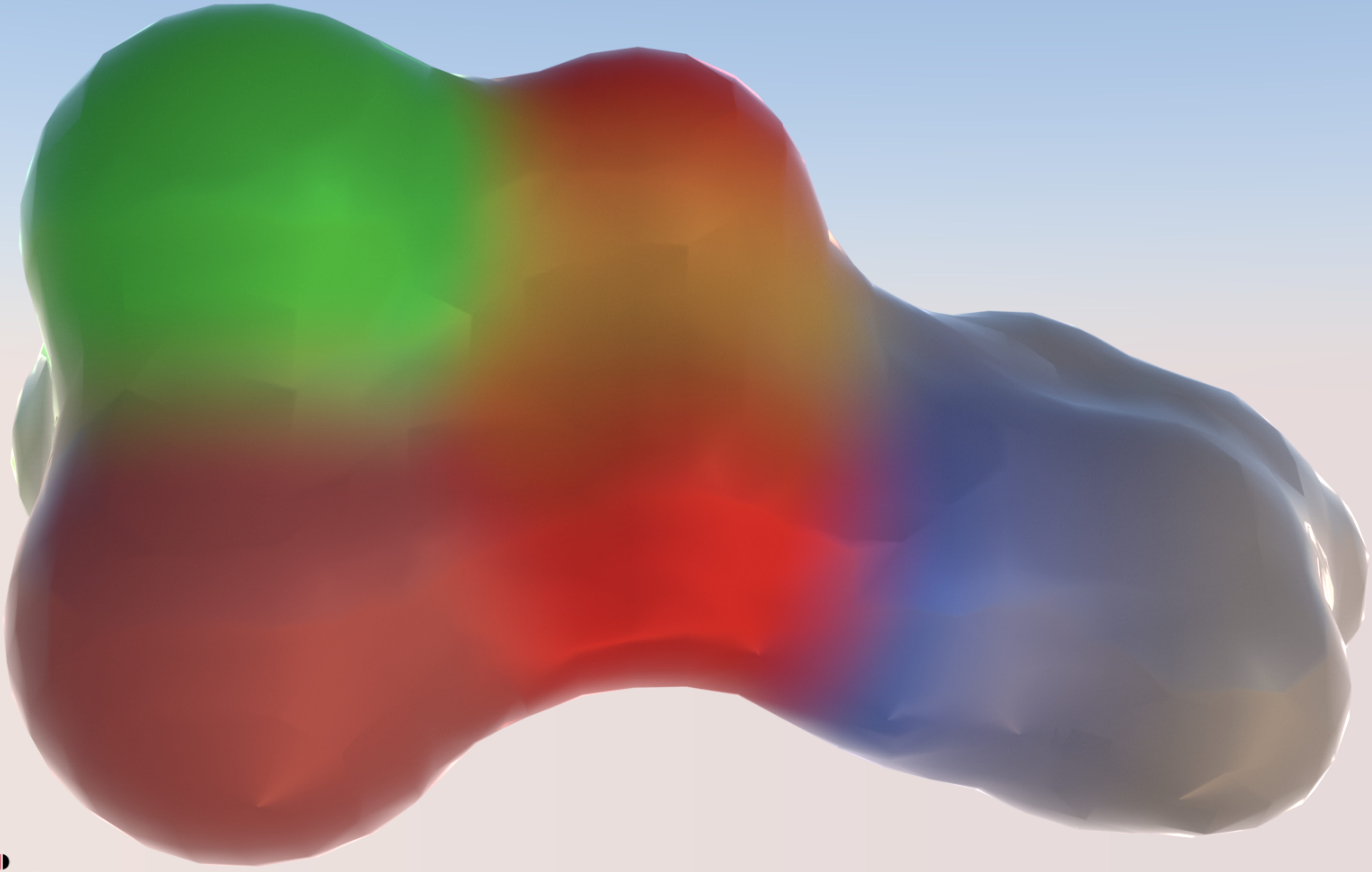

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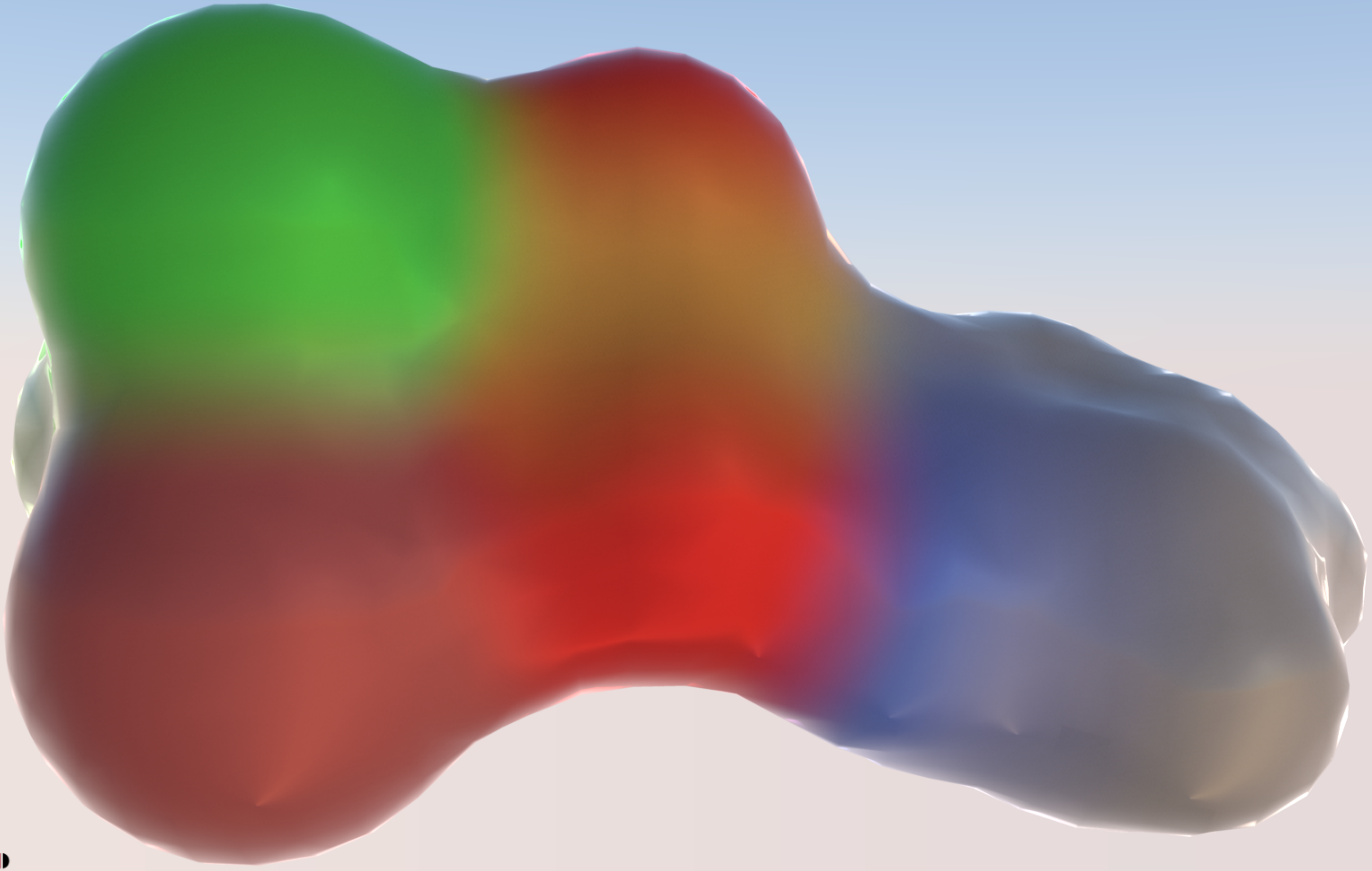
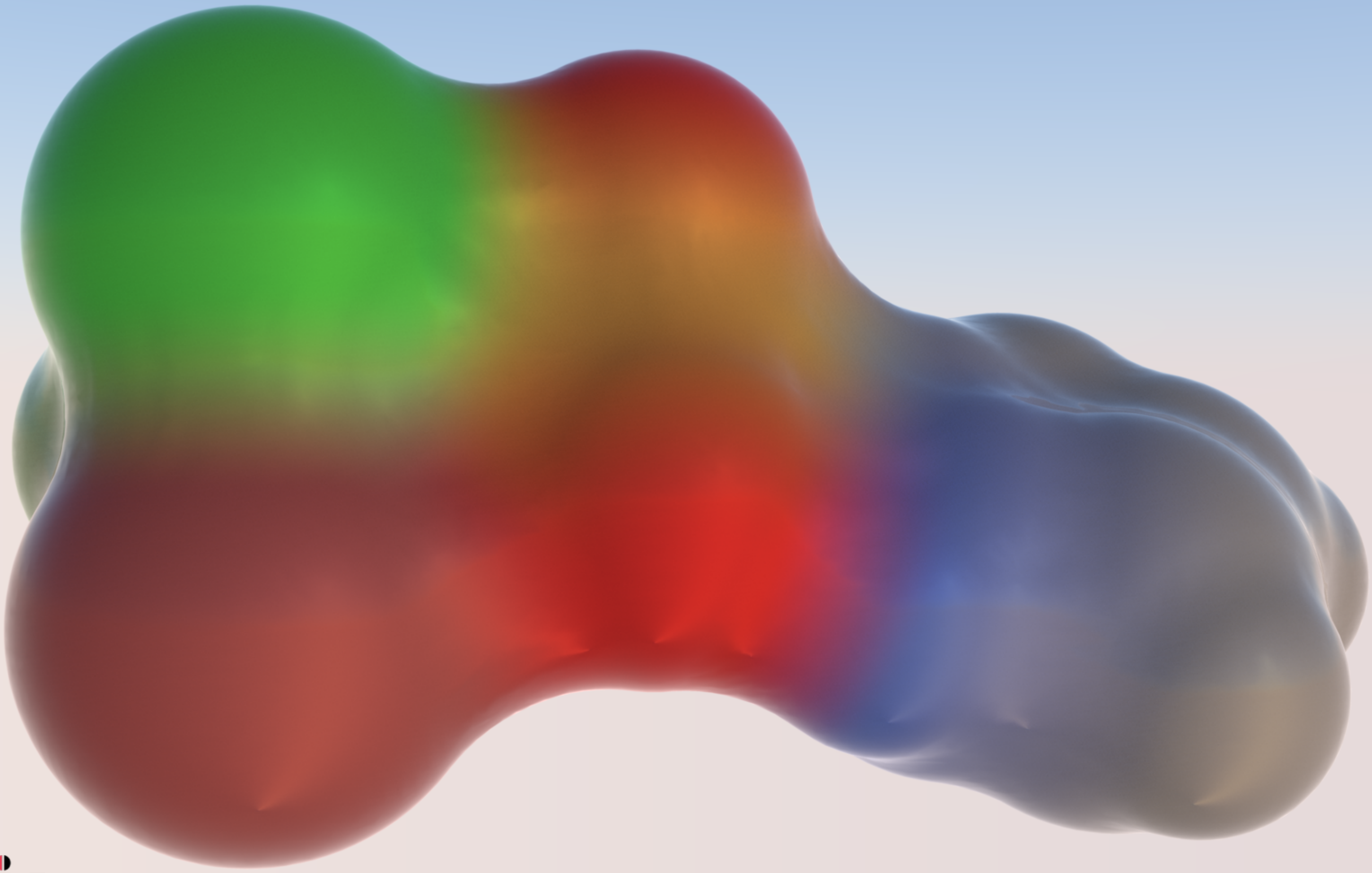
Smooth Marching Cubes



Smooth Marching Cubes With 0.1 Angstrom Resolution



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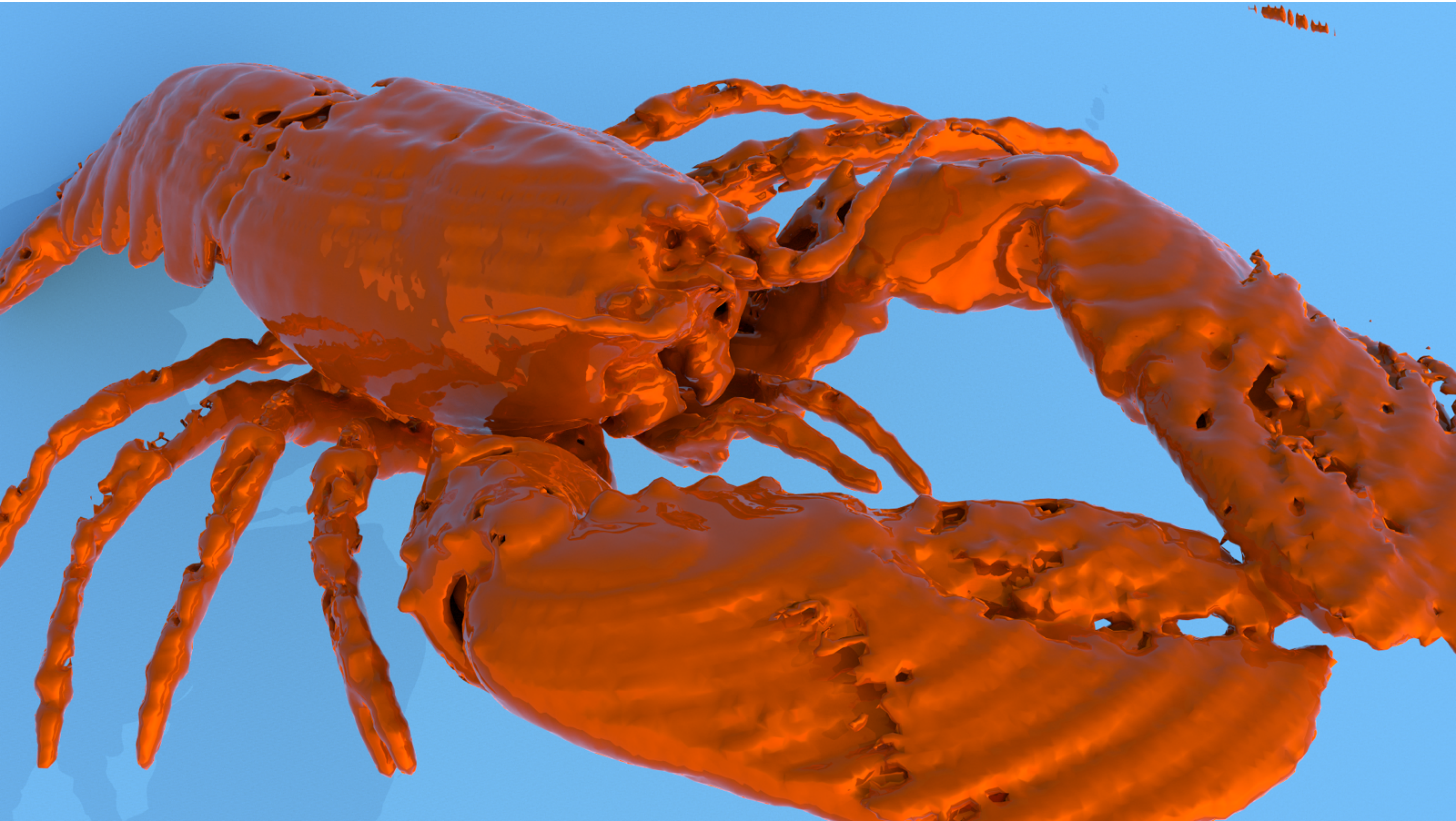
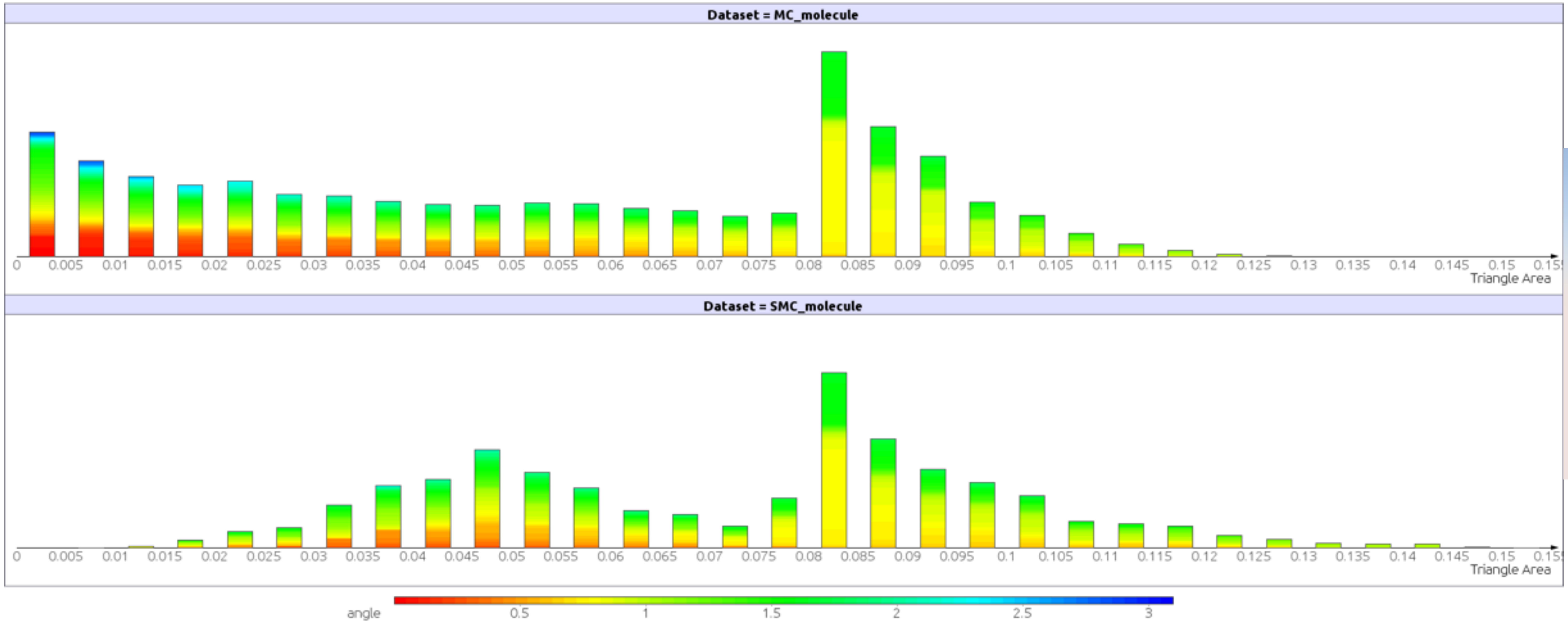
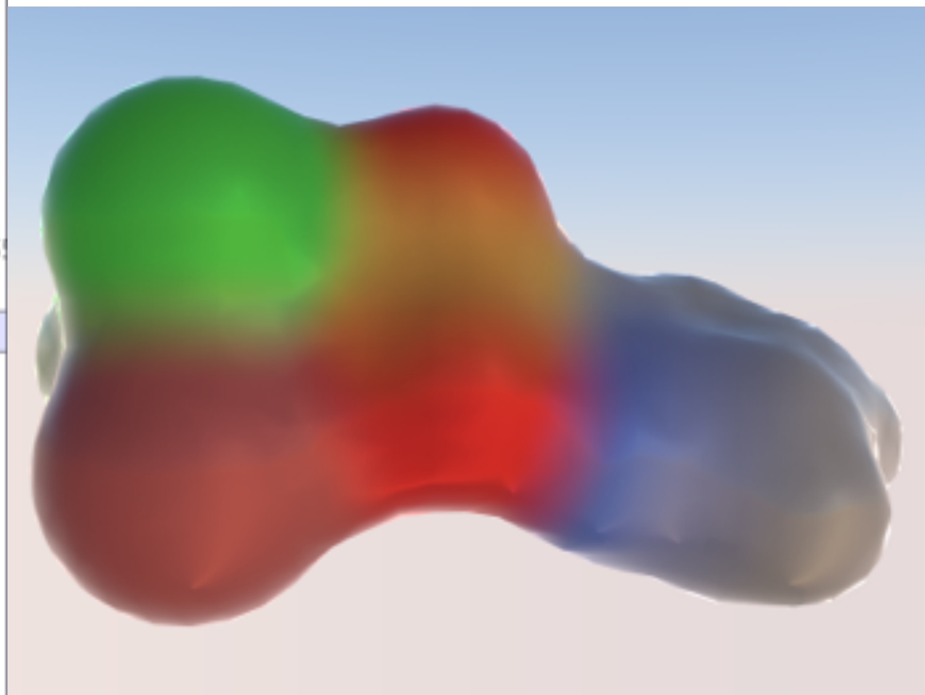
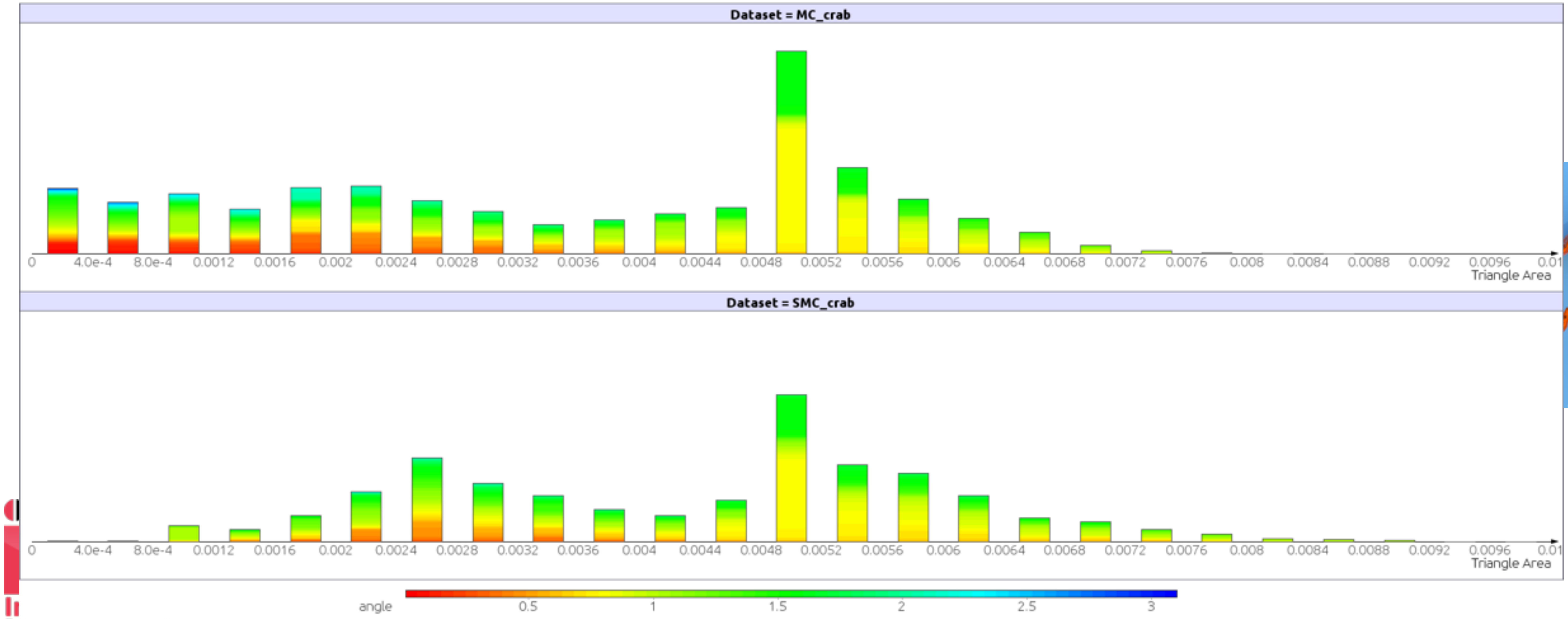
Noisy MRI Dataset: Lobster from volvis.org)
324*301*56 bytes, iso-surface at 40.5
Gives 360038 triangles, 179174 vertexes



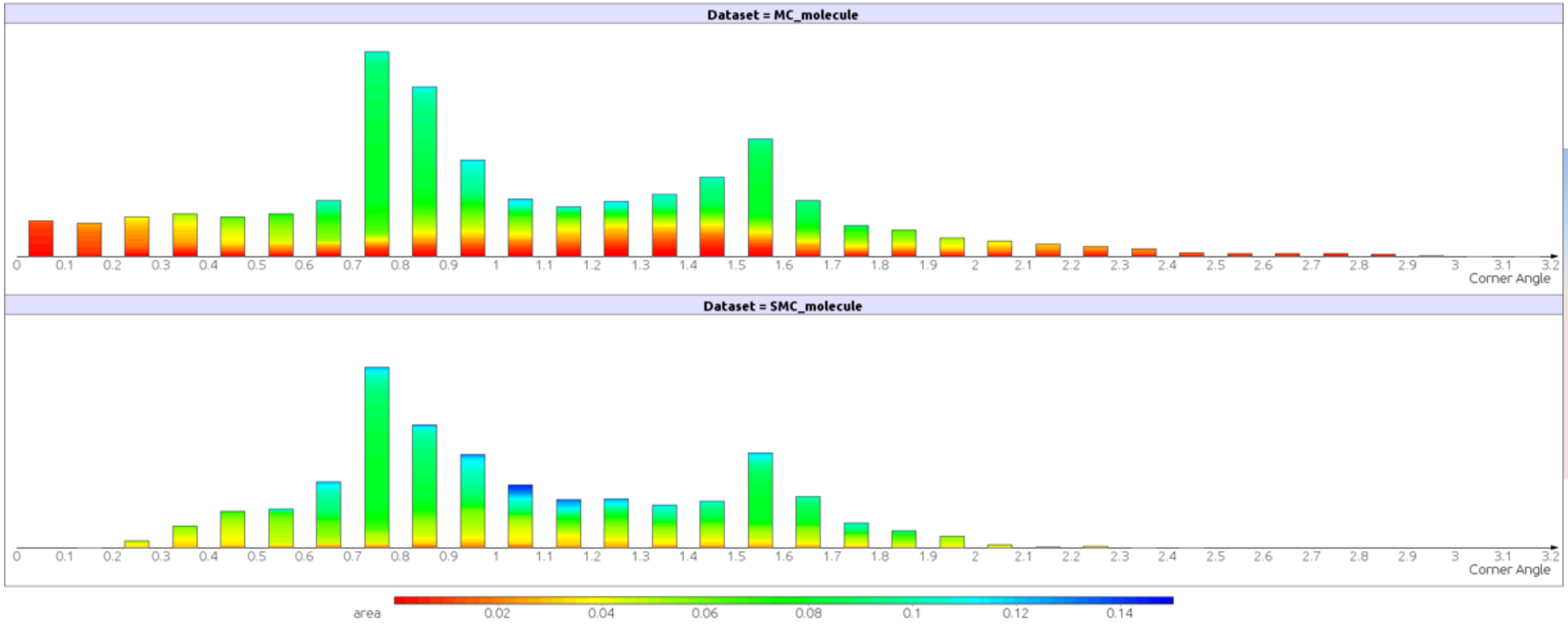
Triangle Area Distribution: MC vs. SMC

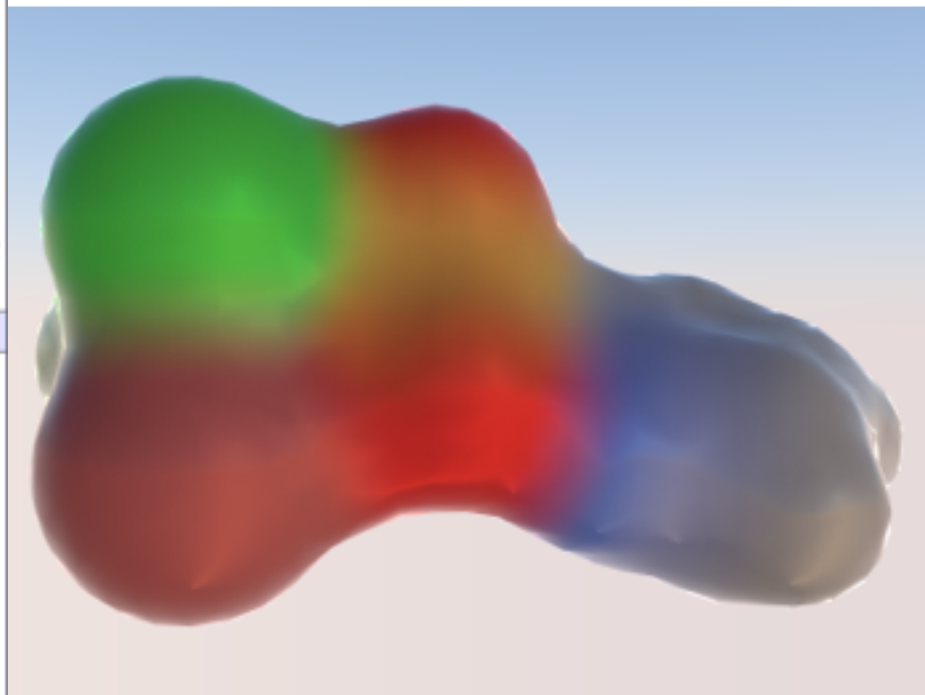


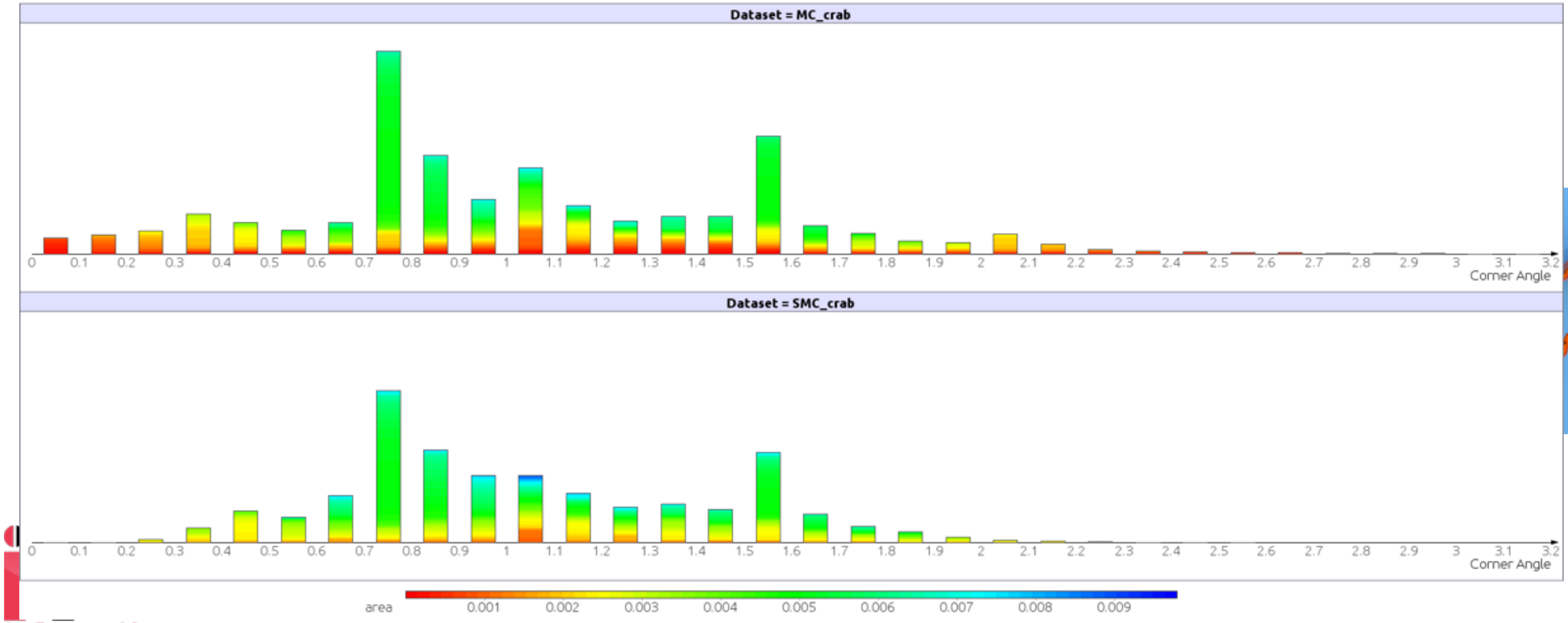




Corner Angle Distribution: MC vs. SMC



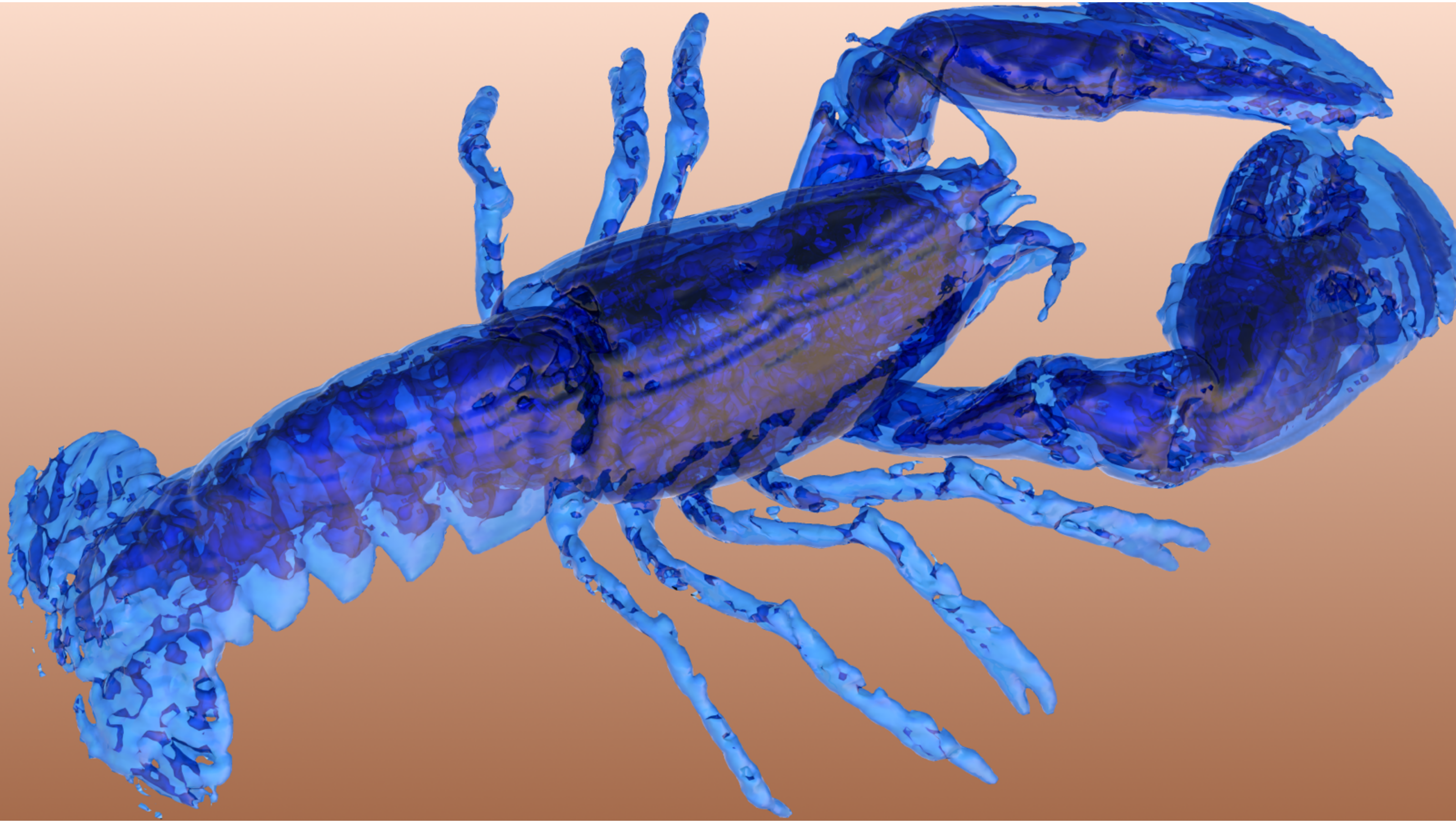




Result

- New method improving the Marching Cubes algorithm
- It entirely avoids small area triangles and, therefore, allows high quality rendering
- There is a very small performance penalty
- 3D Environment independent Java source code
- Robust method applicable for molecular surfaces and noisy data (CT, MRI, etc)

Thank You



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