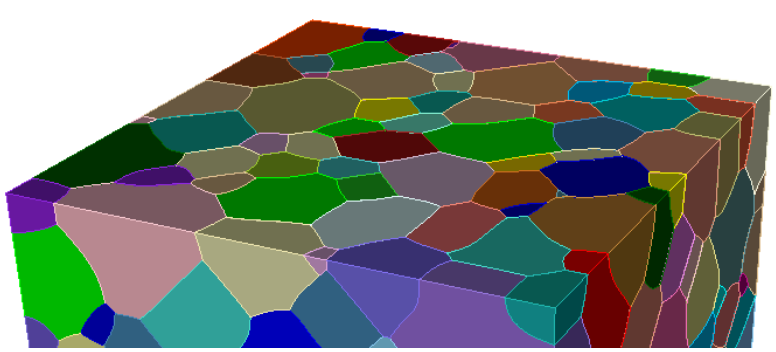
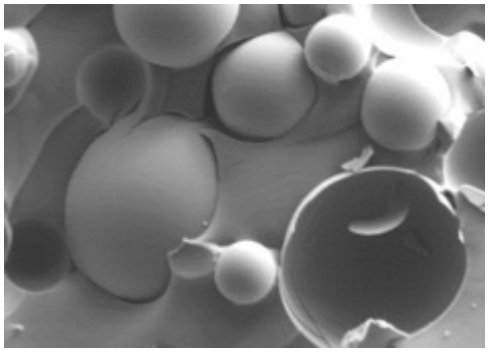
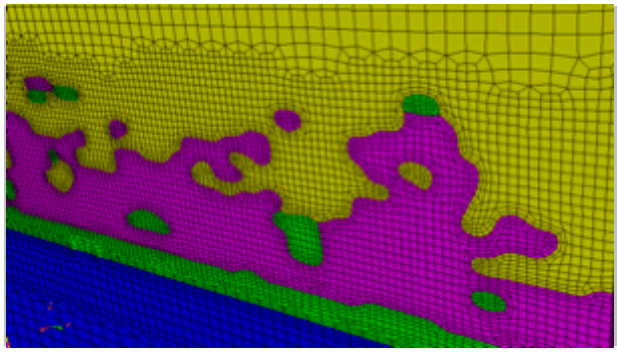
SAND2017-10781C

Barcelona, Spain
Sept 18-21, 2017

Hex Mesh Generation for Computational Materials Modeling

Steven J. Owen, Judith A. Brown, Corey D. Ernst,
Hojun Lim, Kevin N. Long

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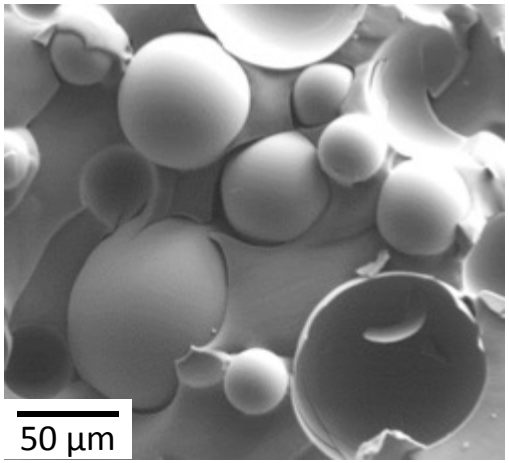
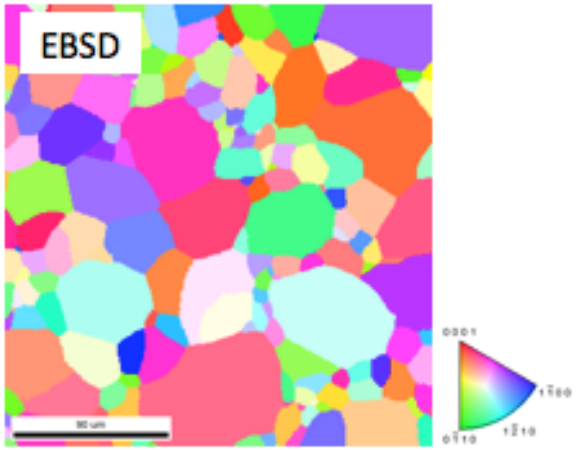
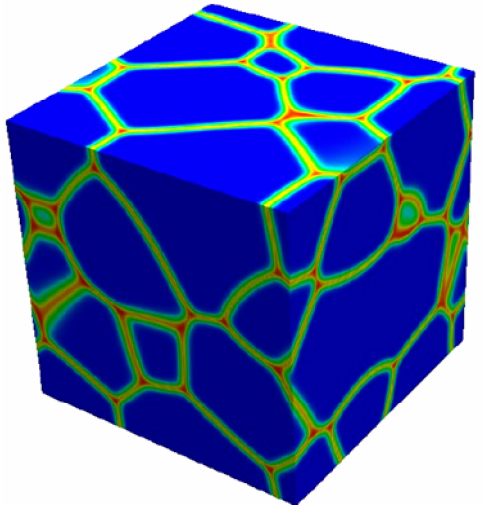
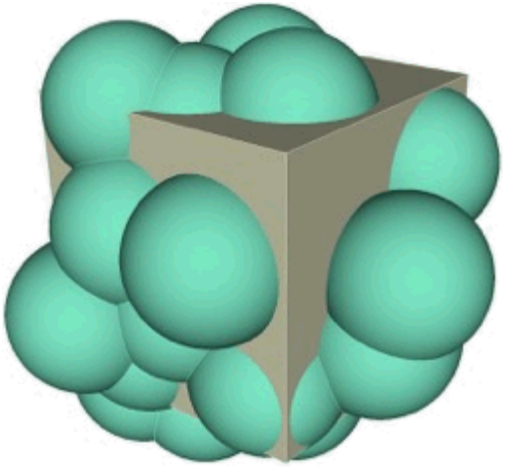
Microstructures

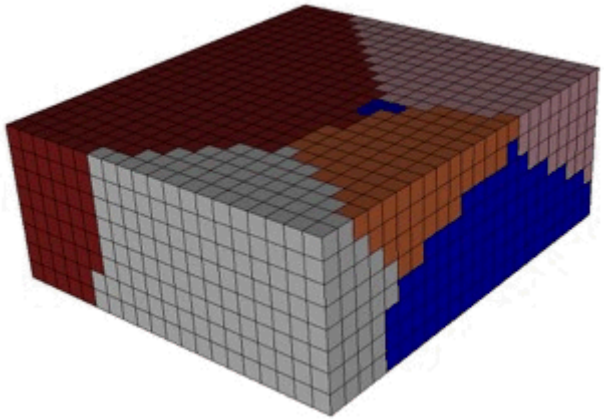








Analytic Geometry

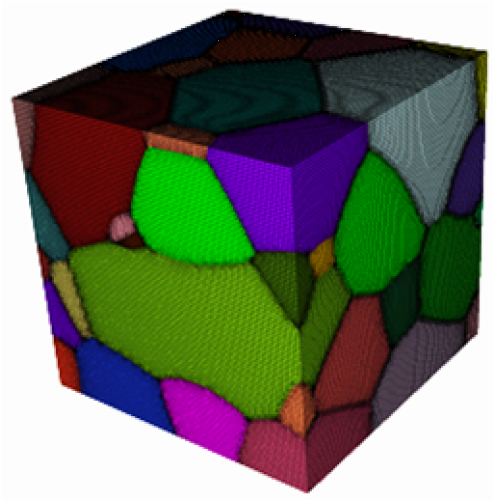


Stair-step Cartesian

$v_A = 0.73$ $v_B = 0.27$	$v_A = 0.41$ $v_B = 0.59$	$v_A = 0.43$ $v_B = 0.57$
$v_A = 0.00$ $v_B = 1.00$	$v_A = 0.55$ $v_B = 0.45$	$v_A = 0.38$ $v_B = 0.62$
$v_A = 0.00$ $v_B = 1.00$	$v_A = 0.79$ $v_B = 0.21$	$v_A = 1.00$ $v_B = 0.00$

Volume Fractions

Mesh Generation



Convert to Volume Fractions

Adapt Grid

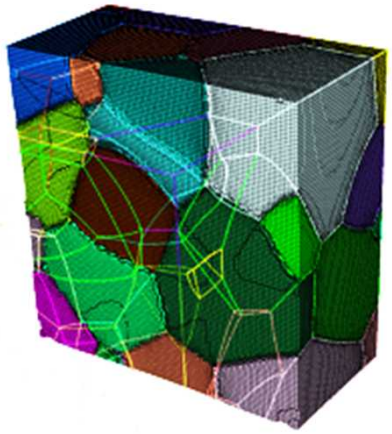
Assign Material

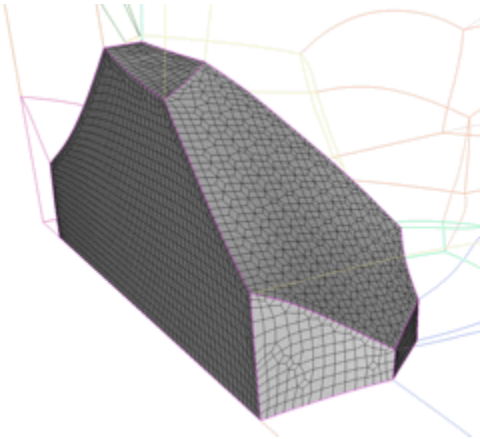
Construct Geometry

Generate Mesh

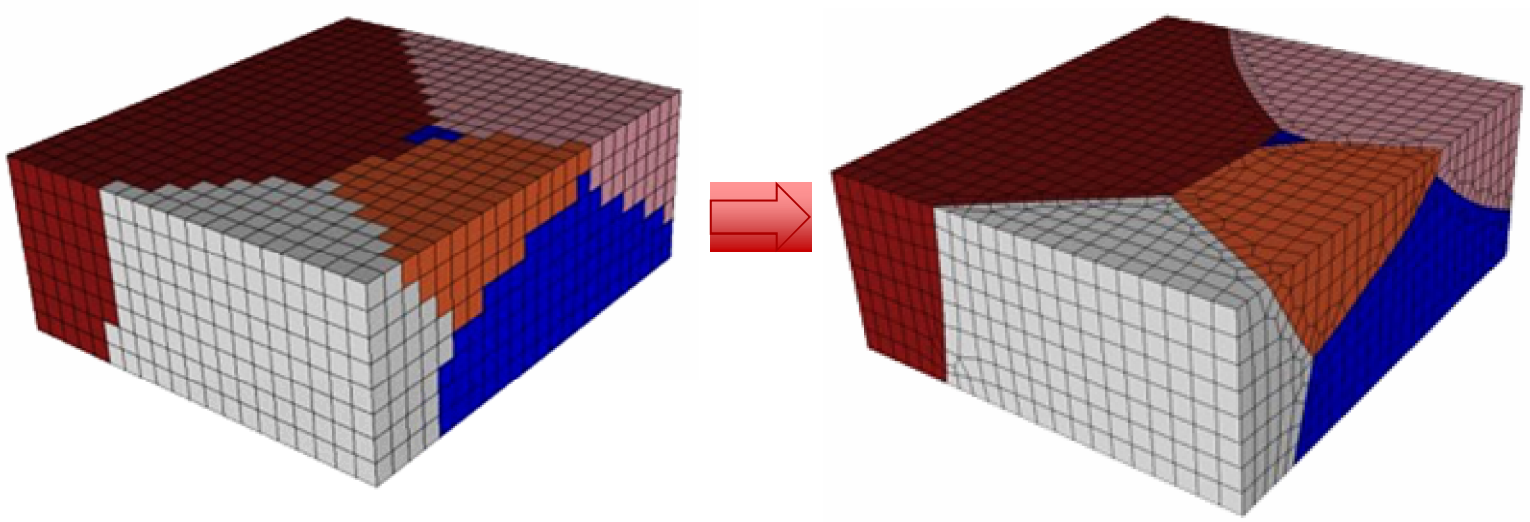
Improve Mesh

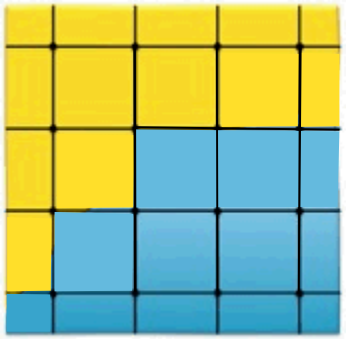
Smooth





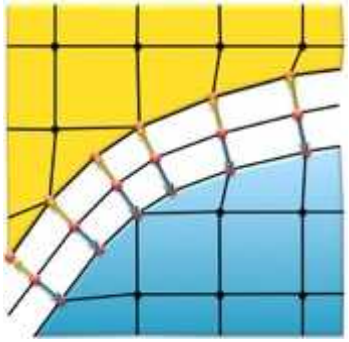
Interface Approximation



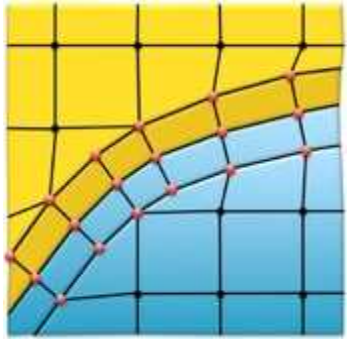


Cartesian Grid with material assignment for each cell

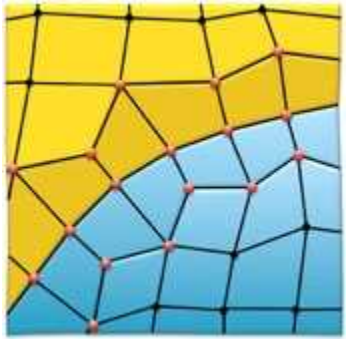
Node locations on interfaces moved



Mesh pulled away from interfaces

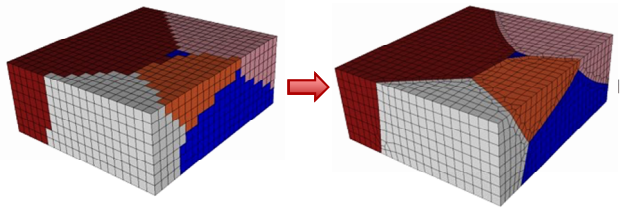


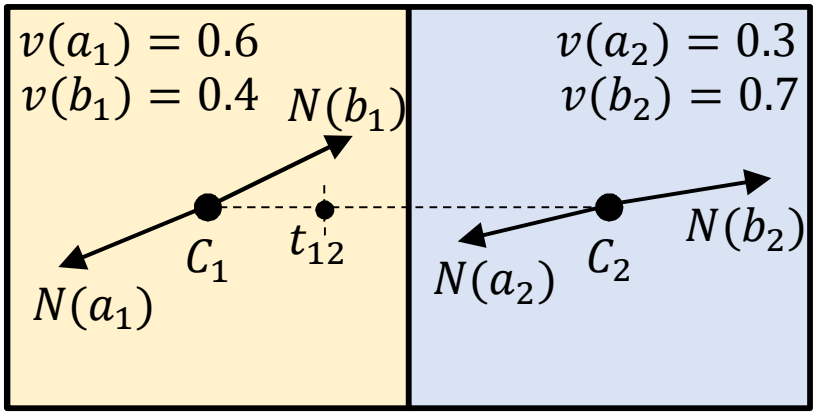
And Layer of hexes inserted

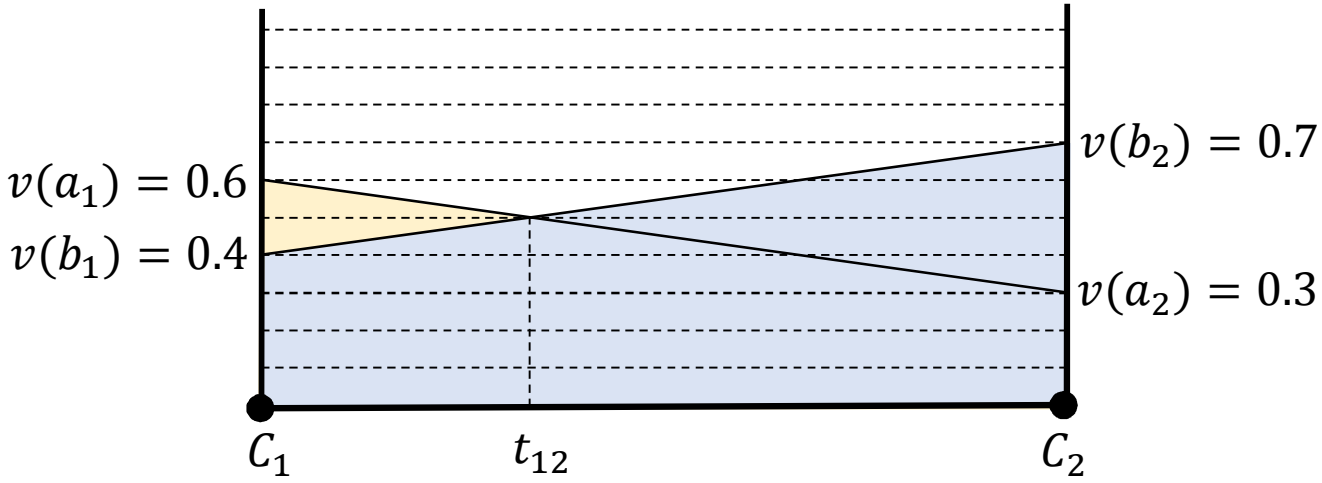


Smoothing performed to improve element quality

Interface Approximation

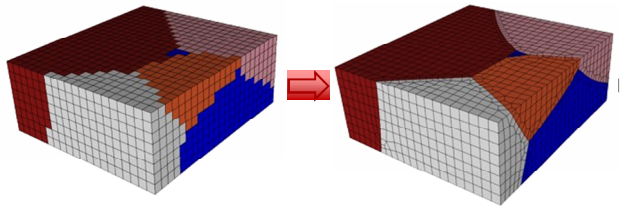


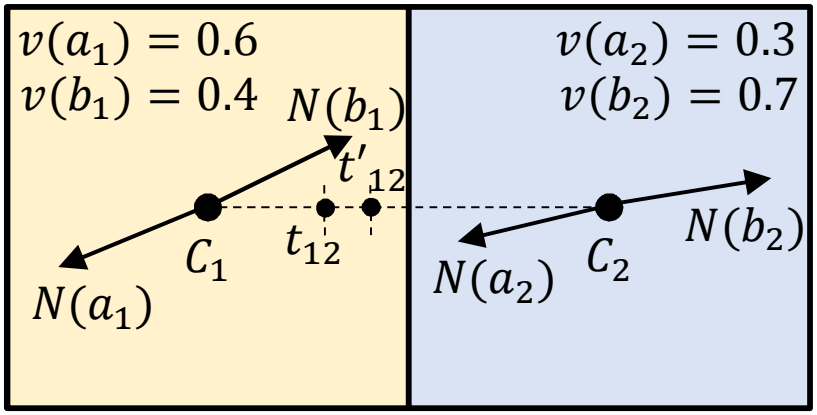


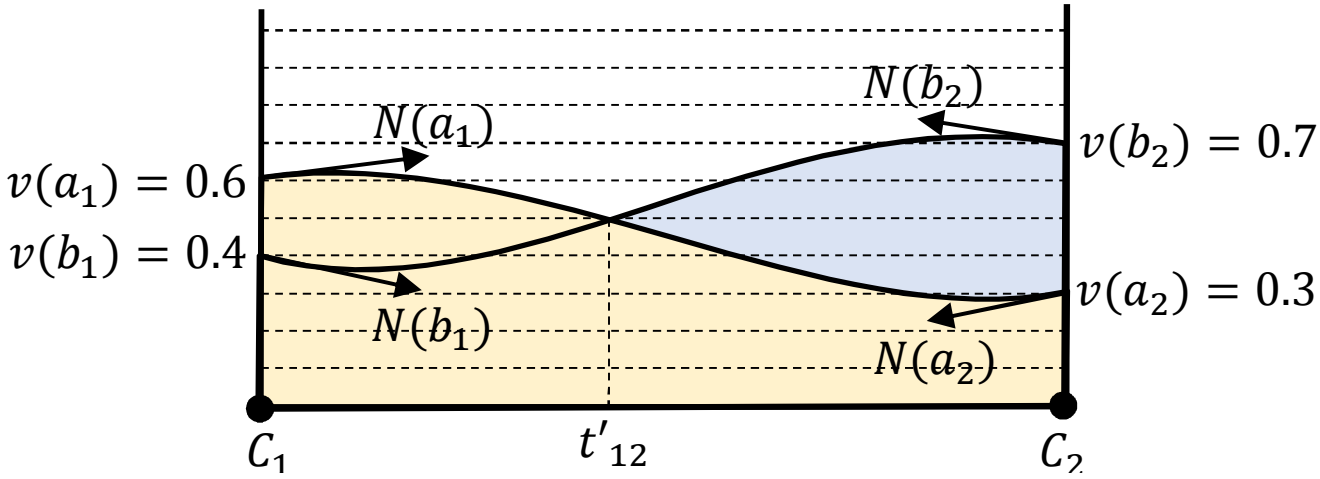


$$t_{12} = \frac{v(b_1) - v(a_1)}{v(a_2) - v(a_1) - v(b_2) + v(b_1)}$$

Interface Approximation

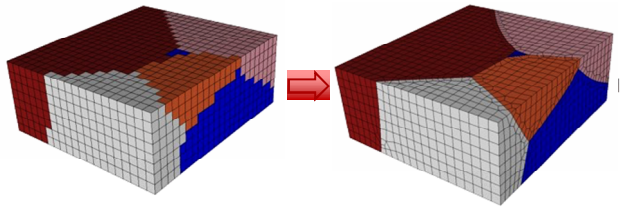


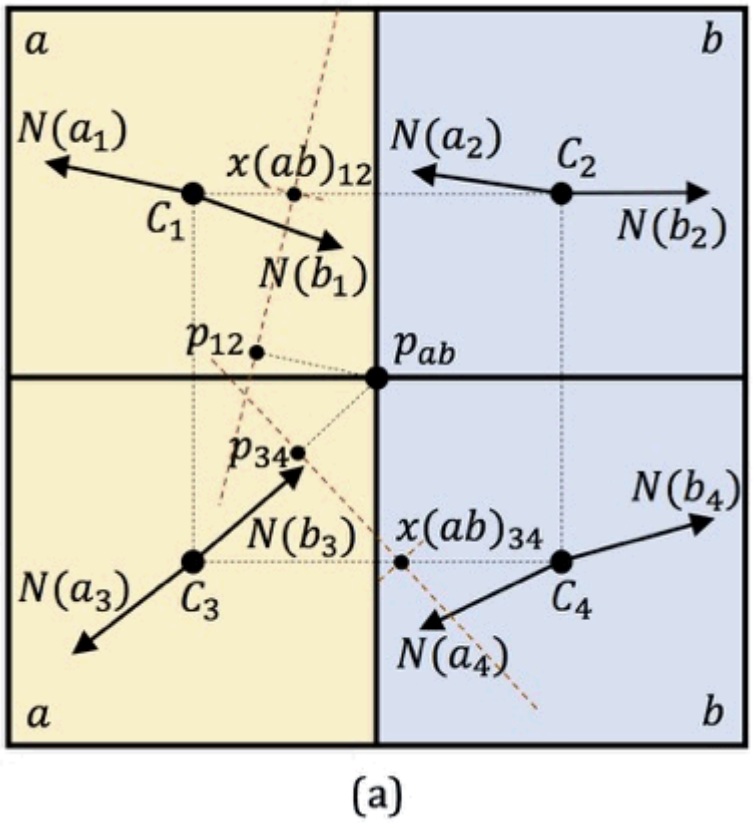




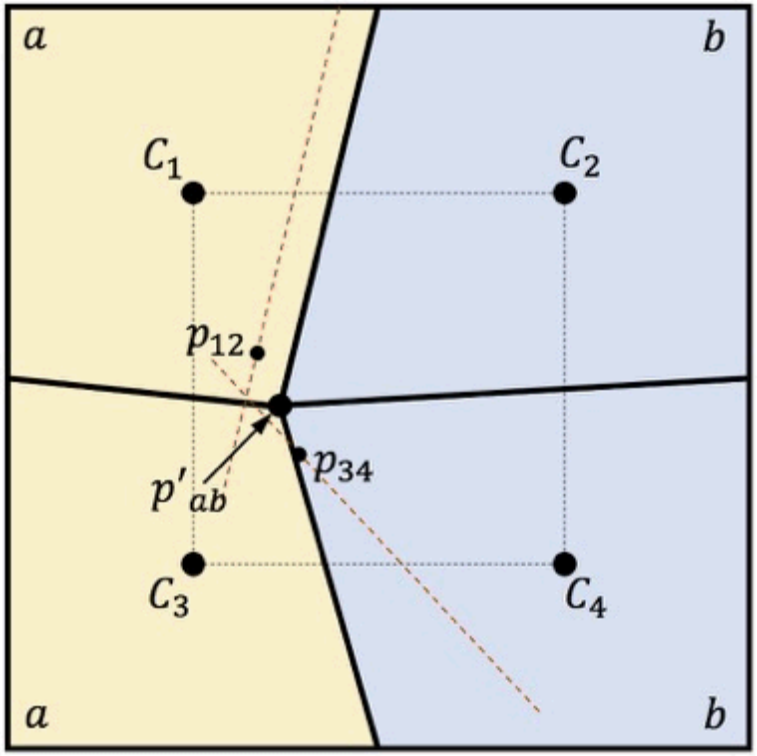
$$a(t) = v(a_1)(2t^3 - 3t^2 + 1) + v(a_2)(-2t^3 + 3t^2) + n(a_1)(t^3 - 2t^2 + t) + n(a_2)(t^3 - t^2)$$
$$b(t) = v(b_1)(2t^3 - 3t^2 + 1) + v(b_2)(-2t^3 + 3t^2) + n(b_1)(t^3 - 2t^2 + t) + n(b_2)(t^3 - t^2)$$

Interface Approximation





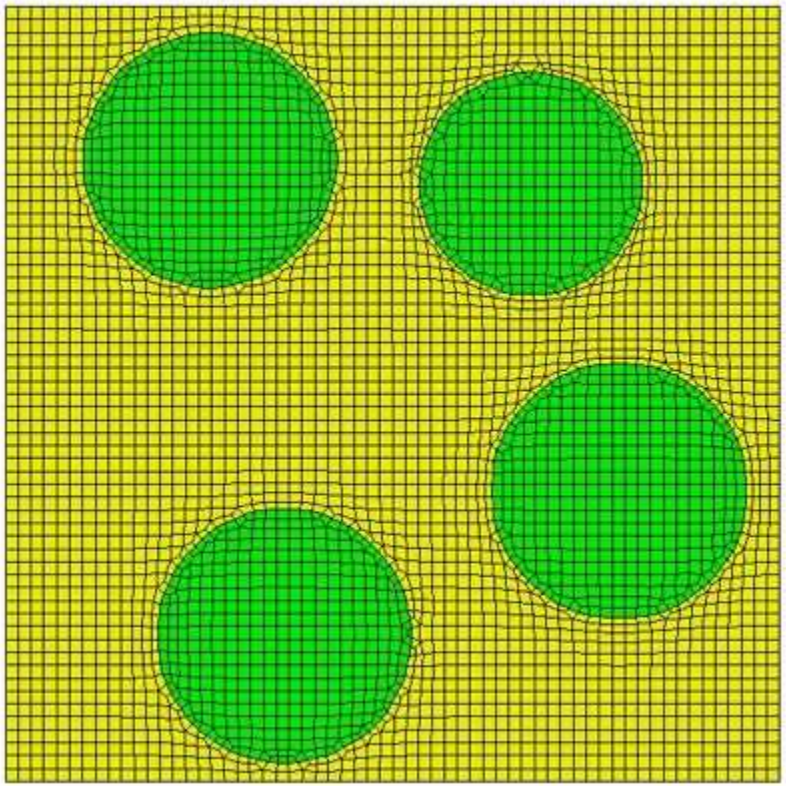
(a)

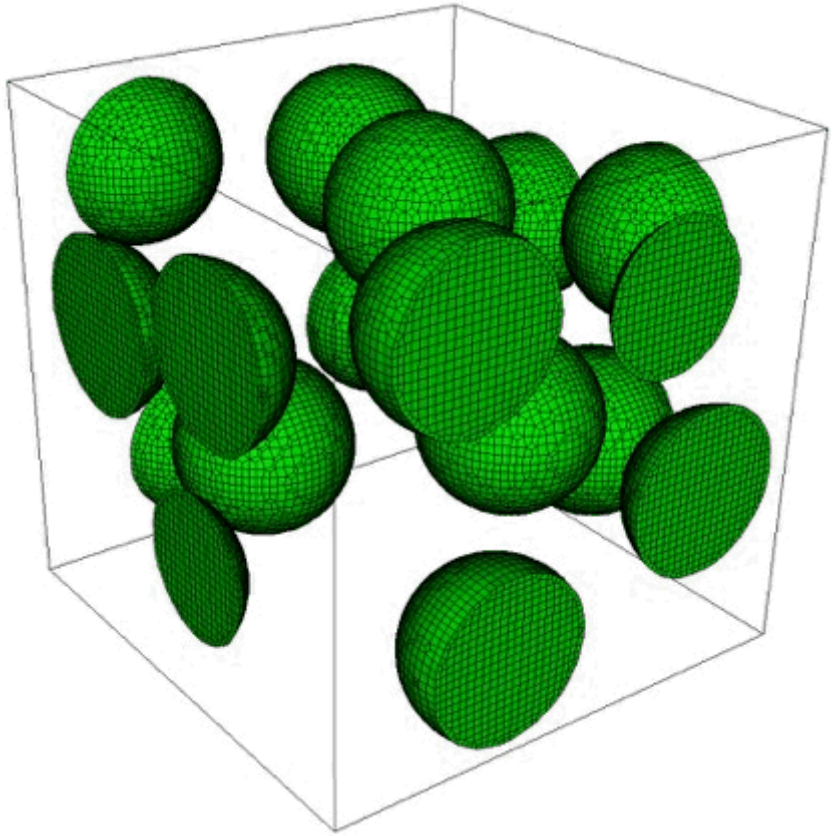


(b)

Example

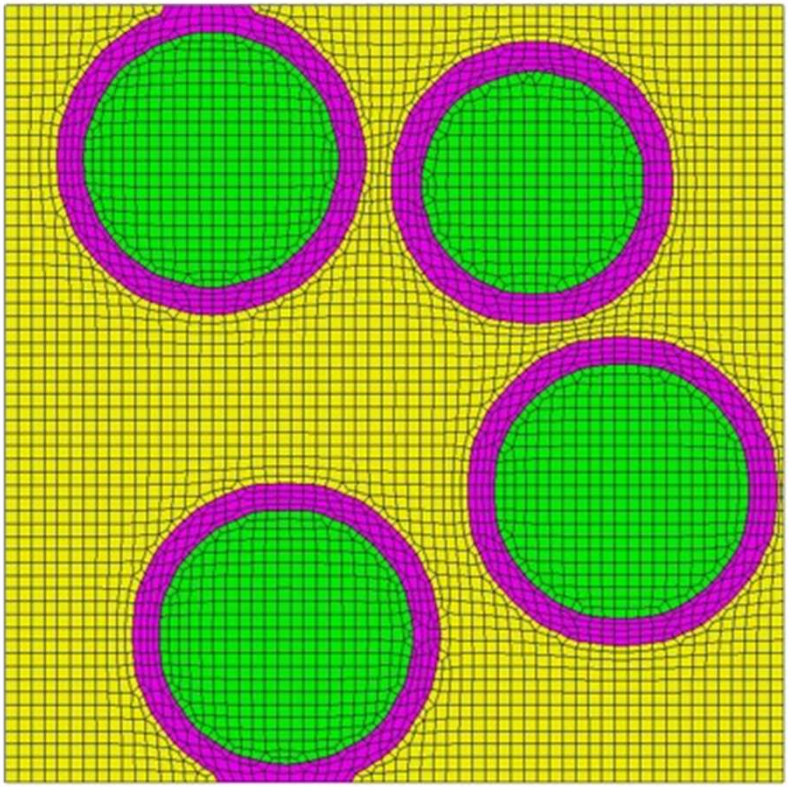
Spherical particles

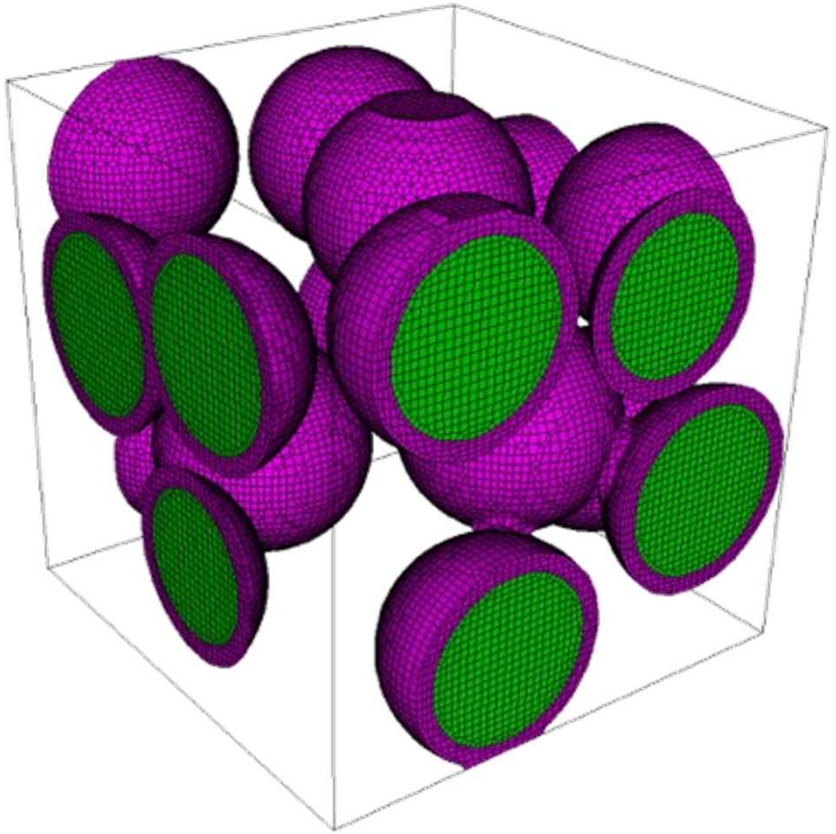




Example

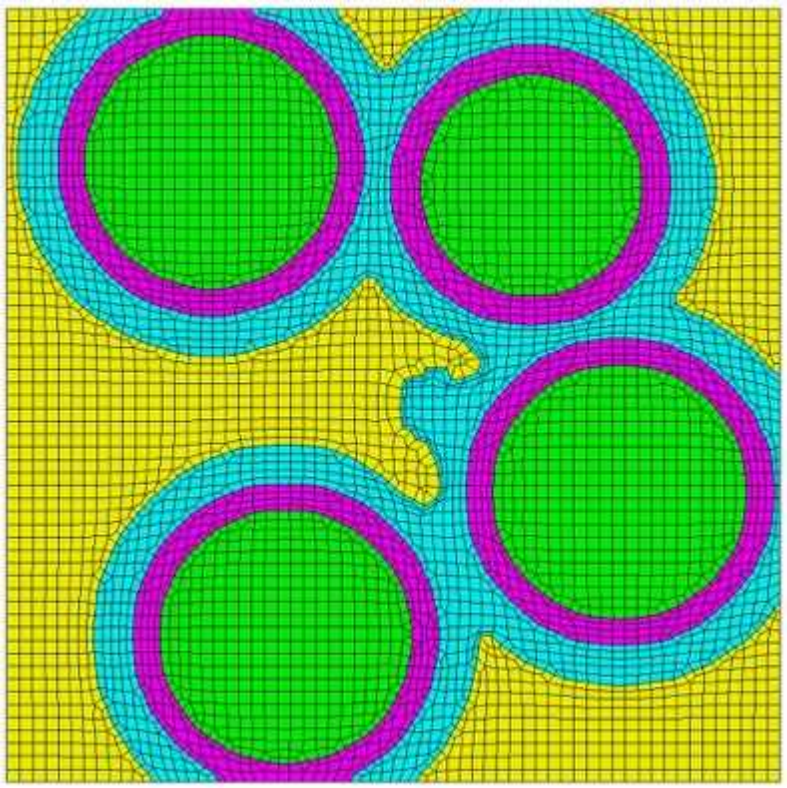
Spherical particles

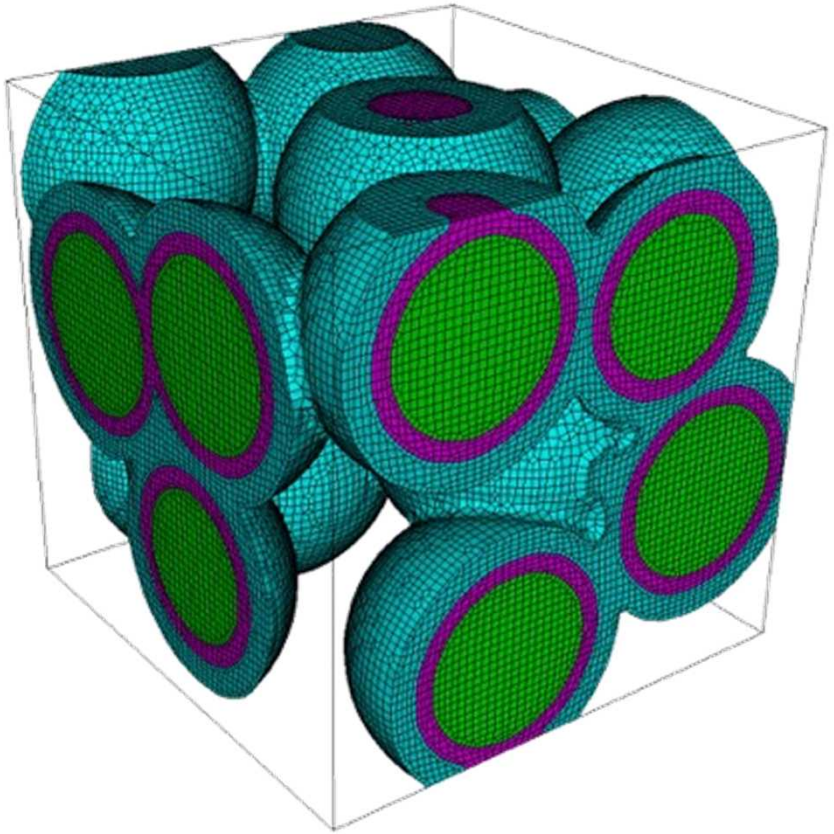




Example

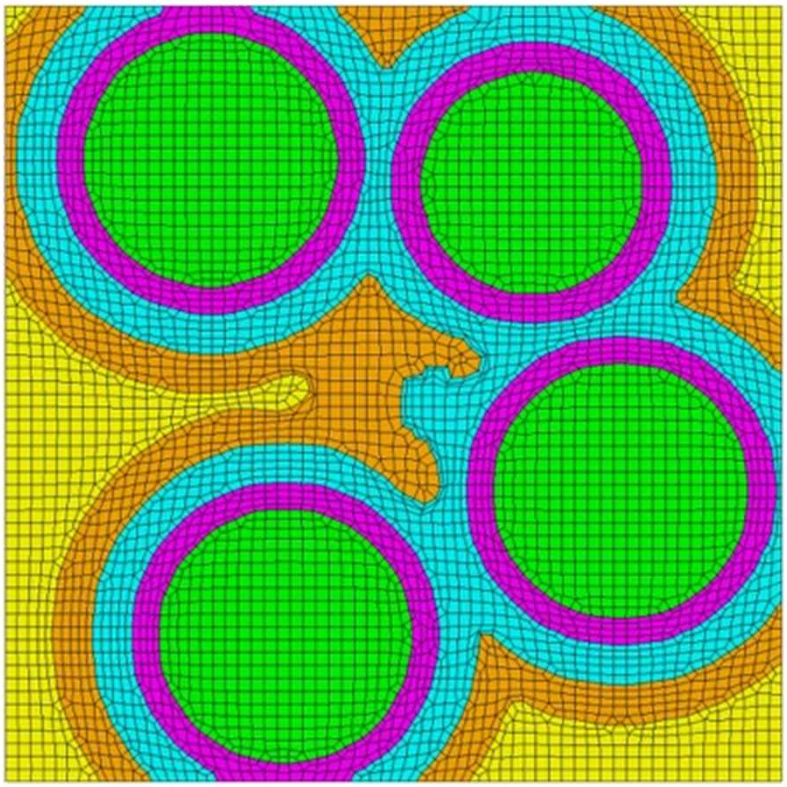
Spherical particles

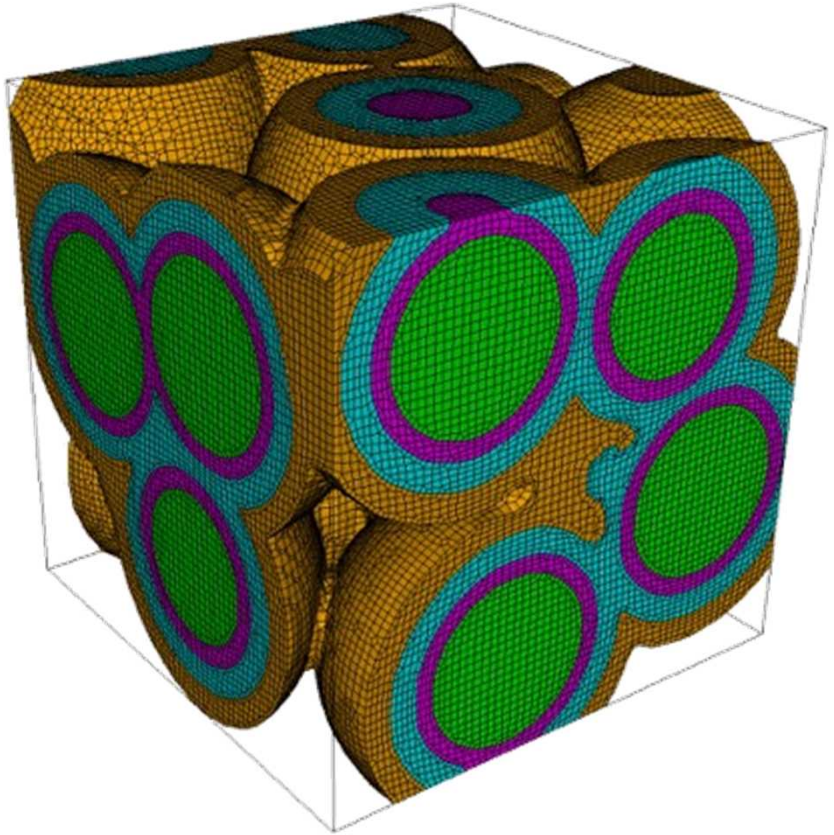




Example

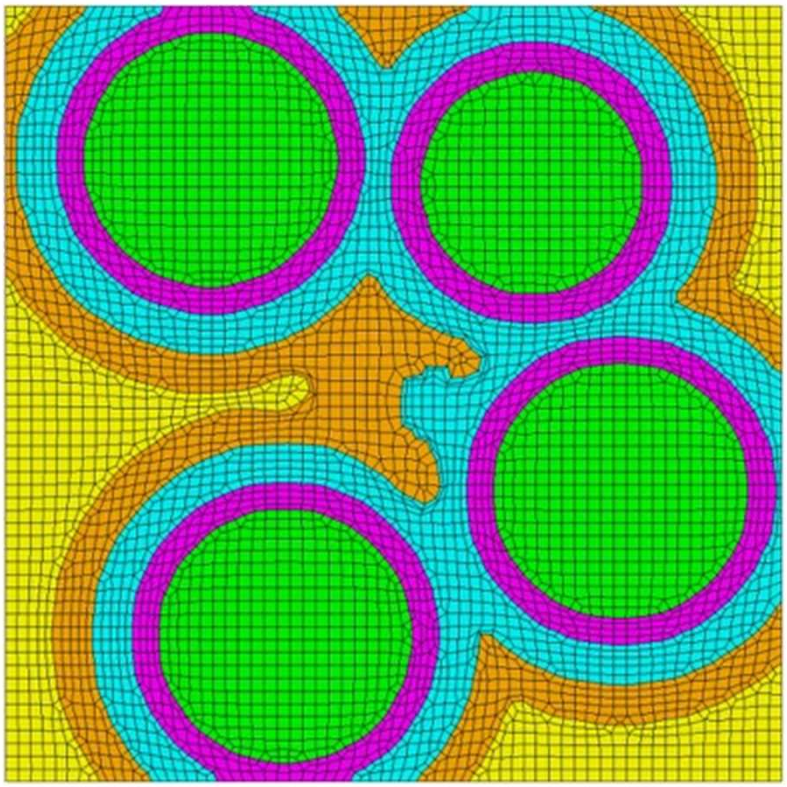
Spherical particles

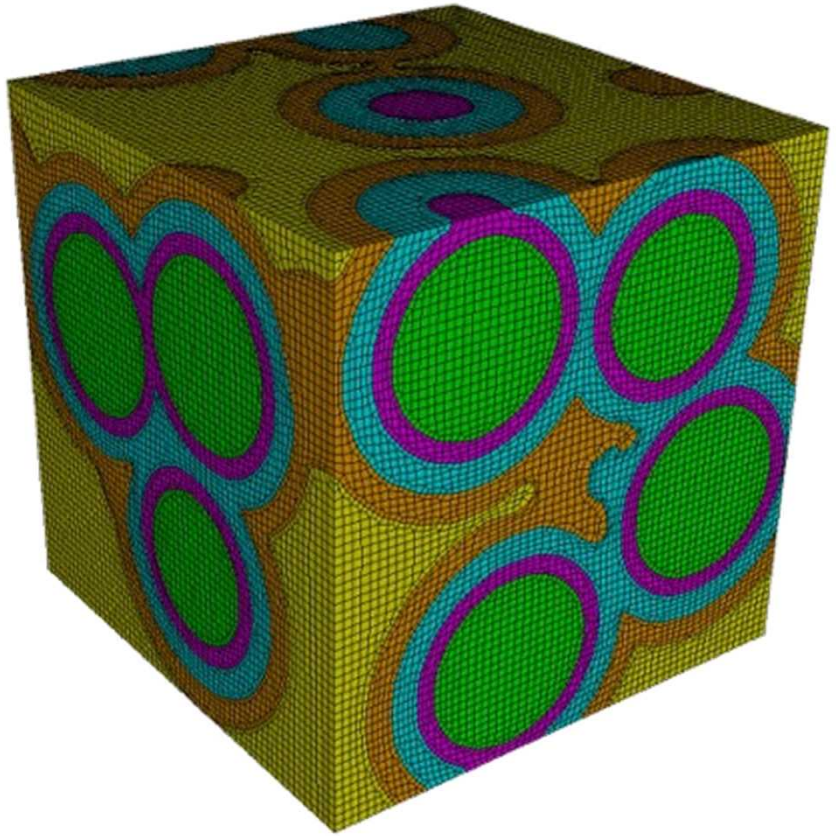




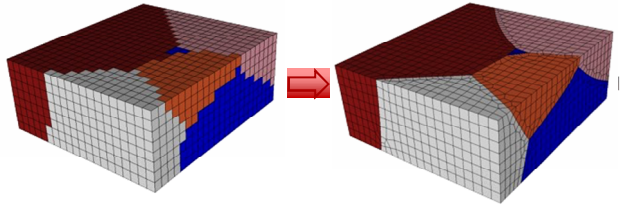
Example

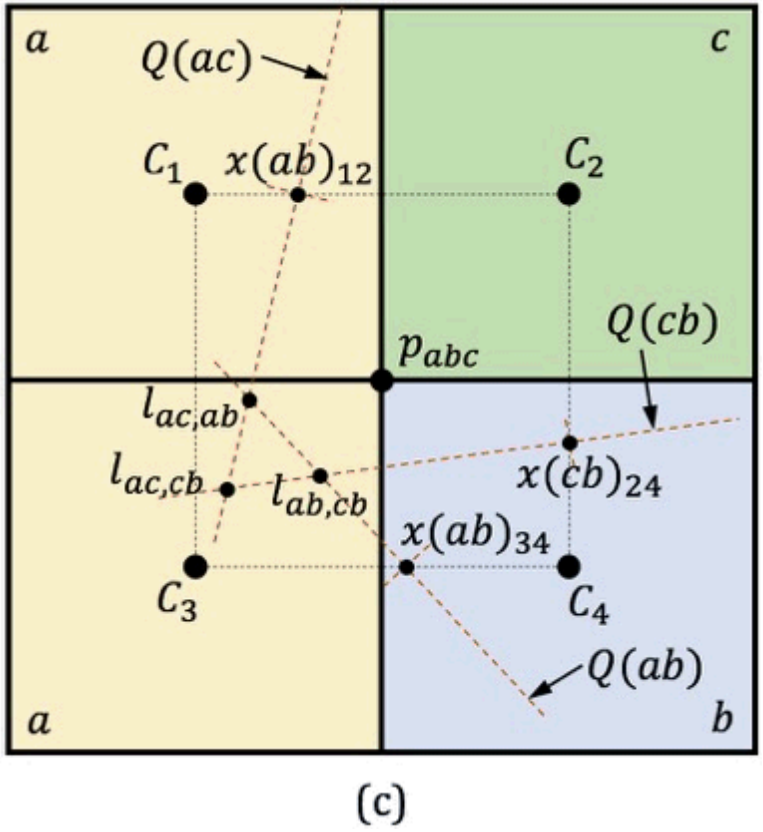
Spherical particles



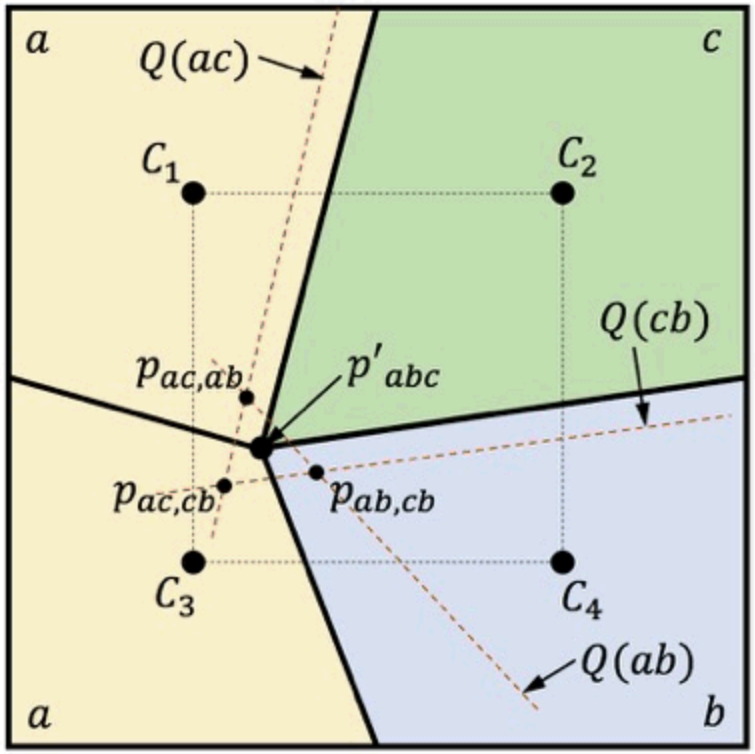


Interface Approximation



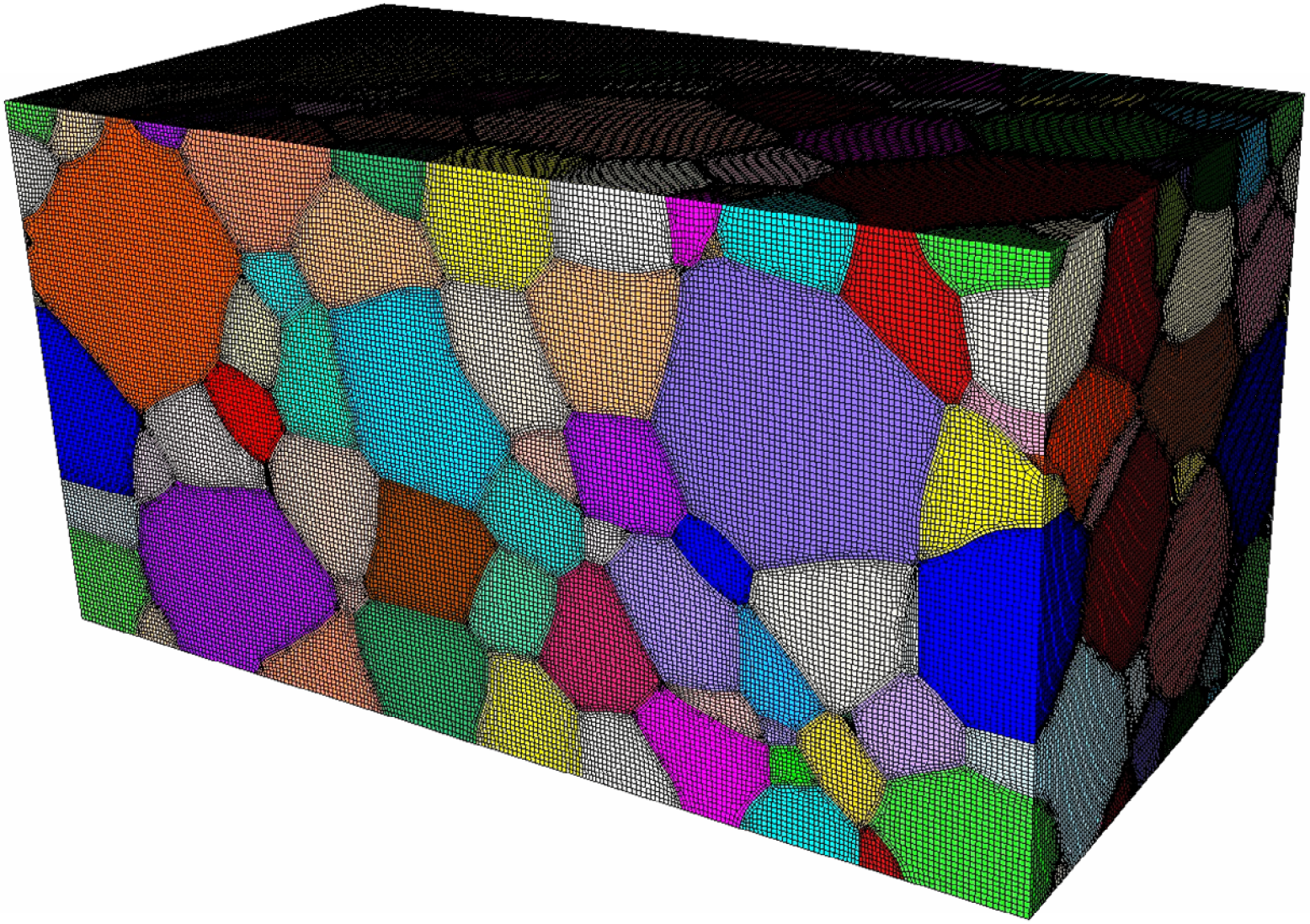


(c)

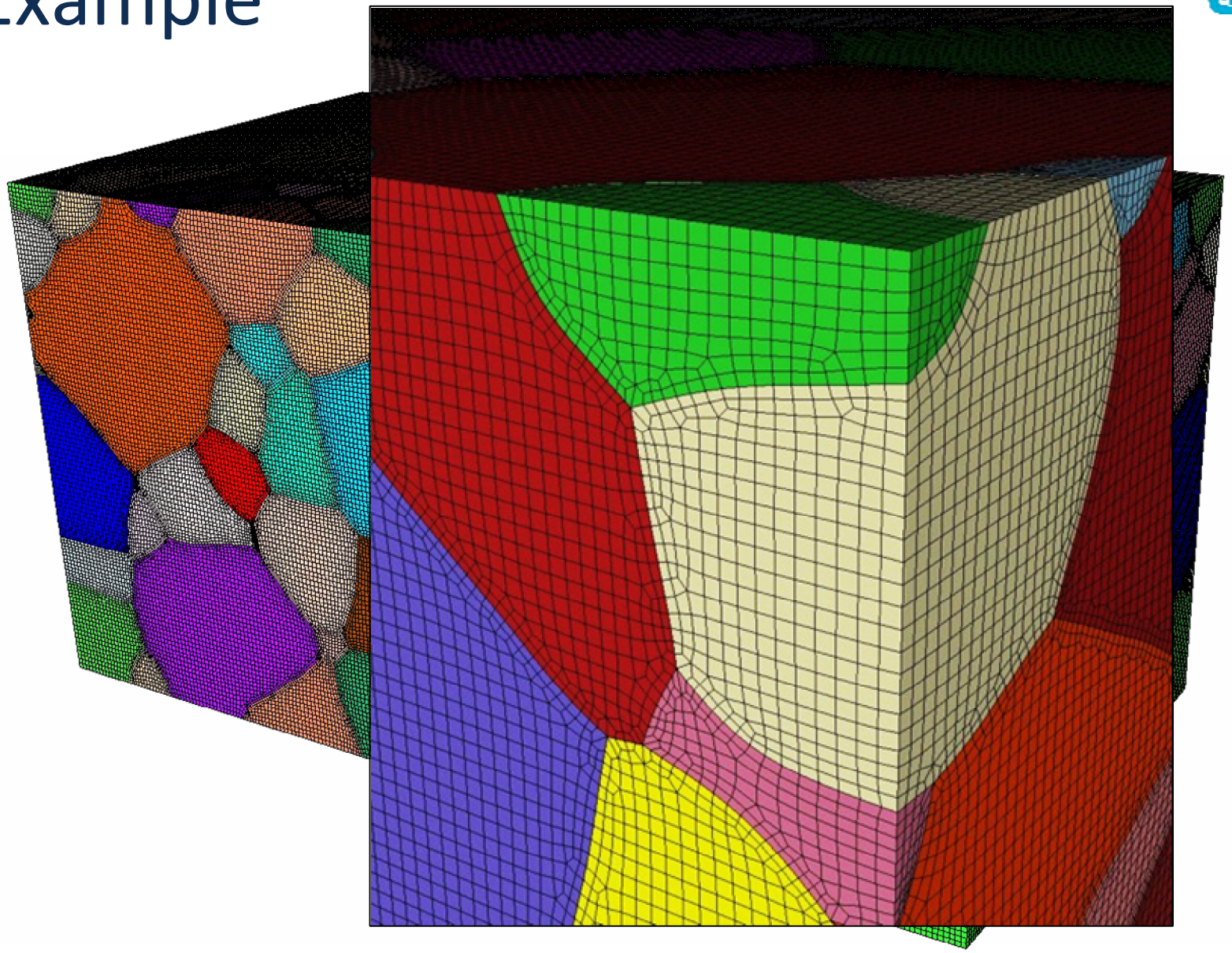


(d)

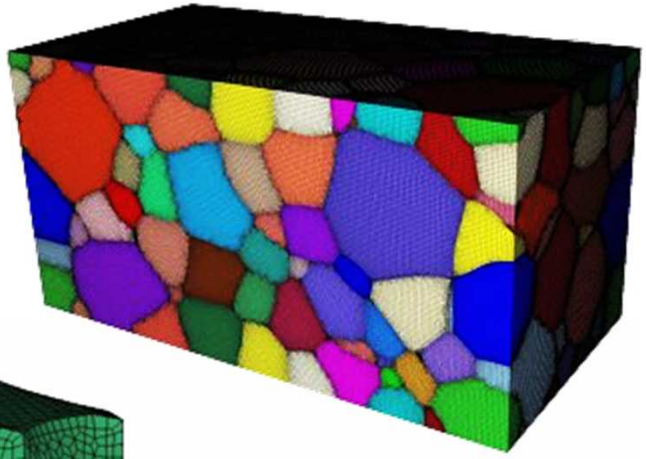
Example

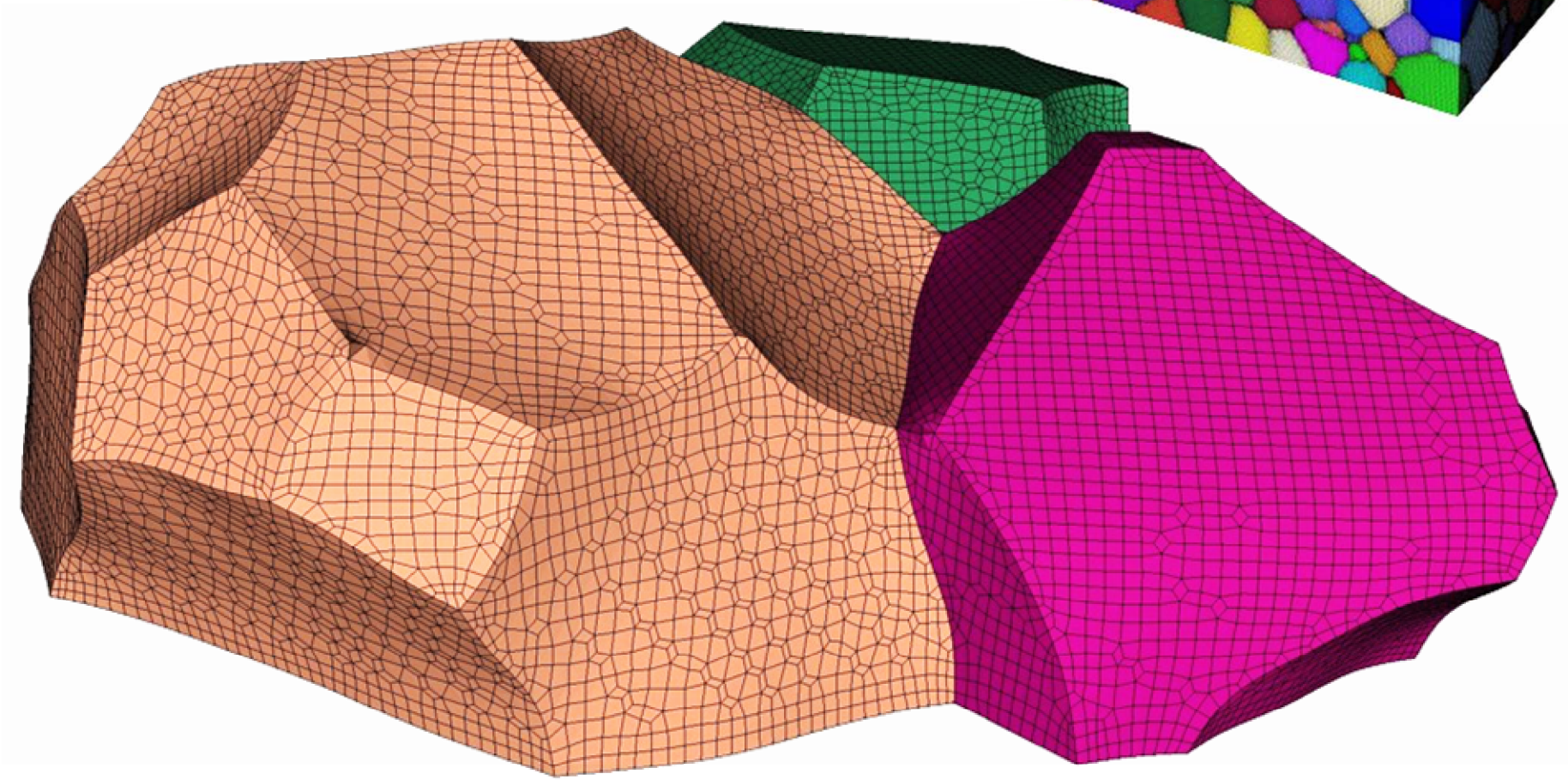


Example

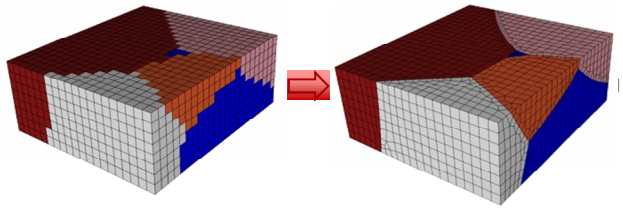


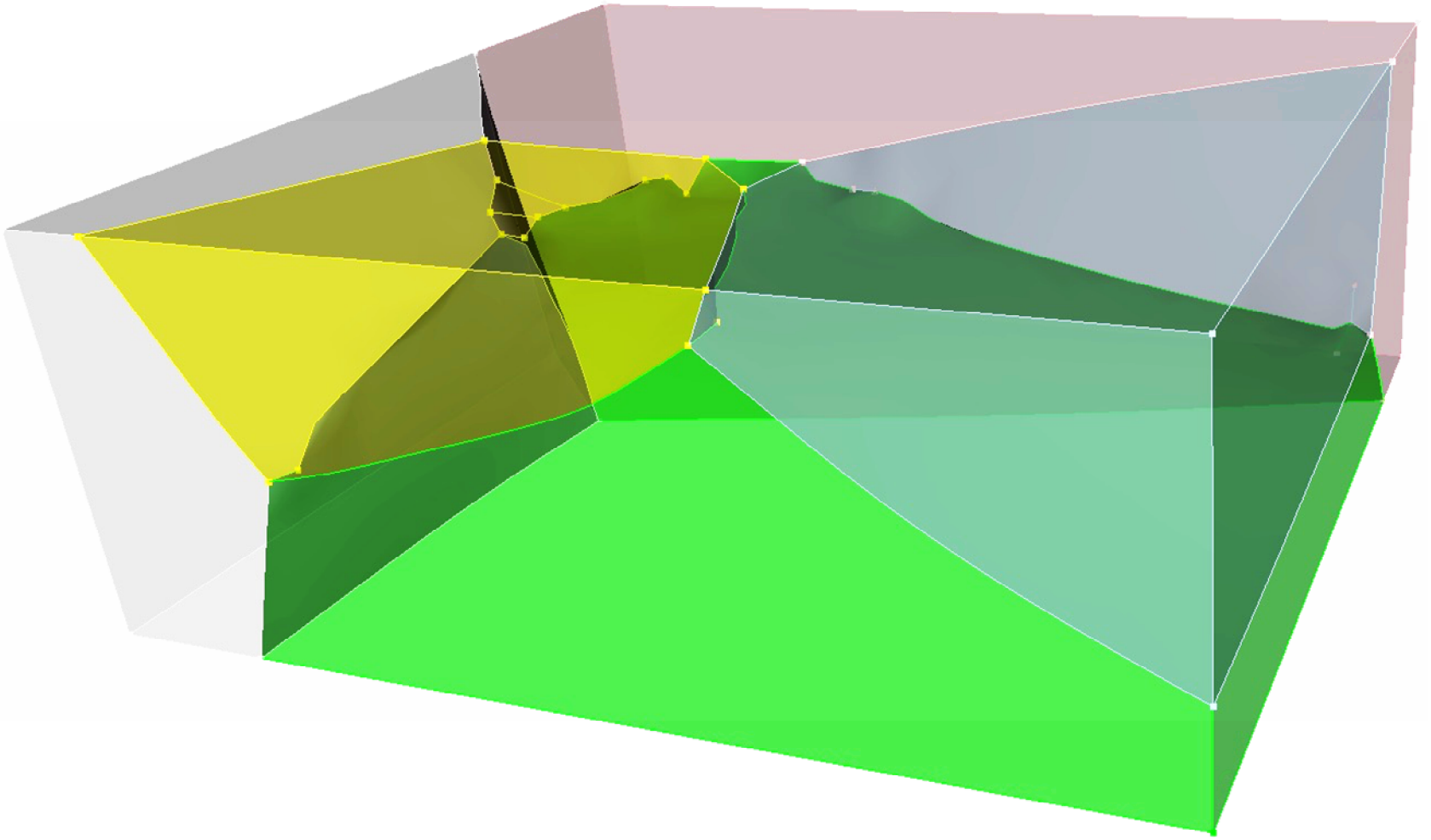
Example





Pillowing





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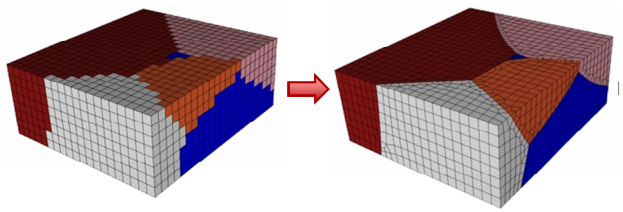
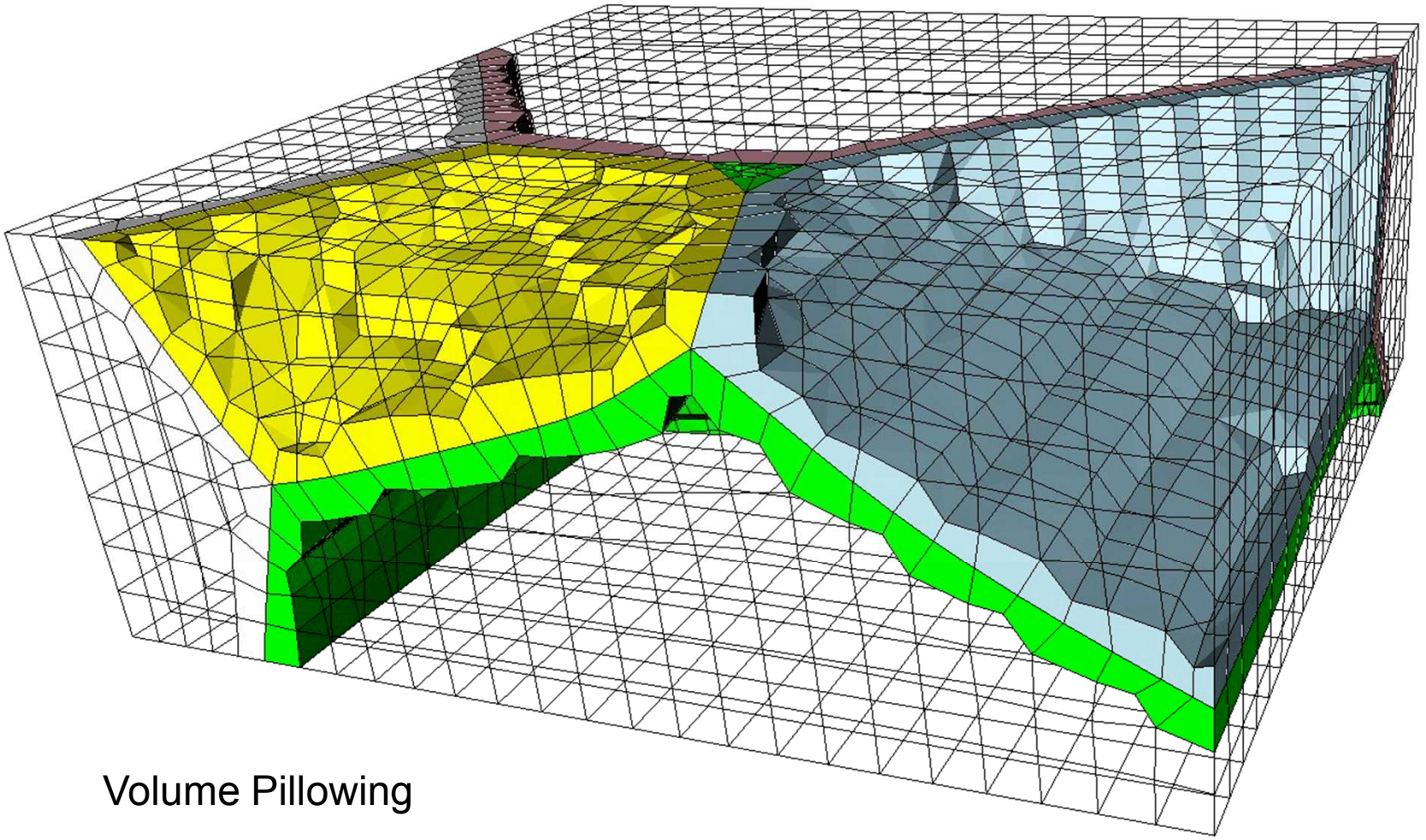
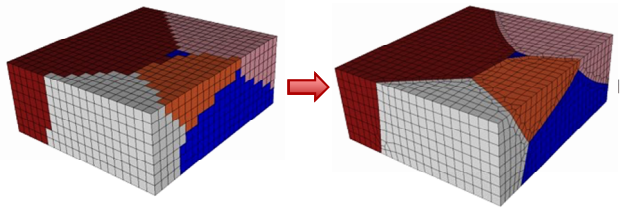
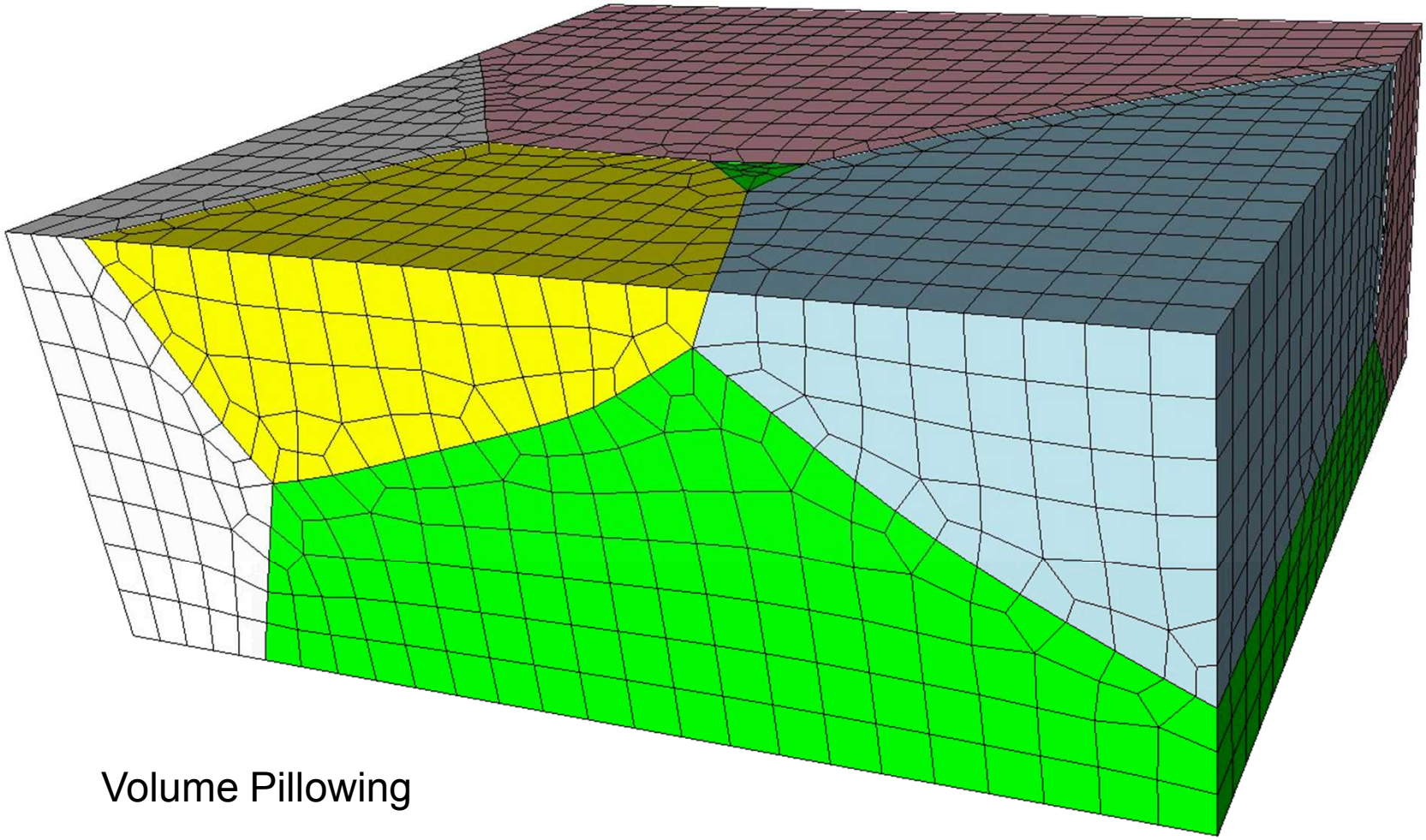




Volume Pillowing

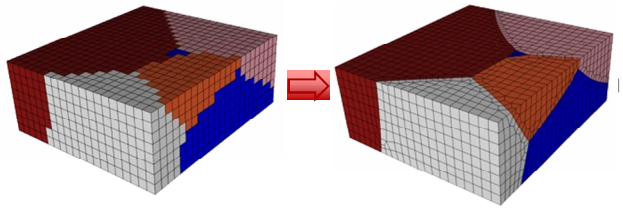
Pillowing

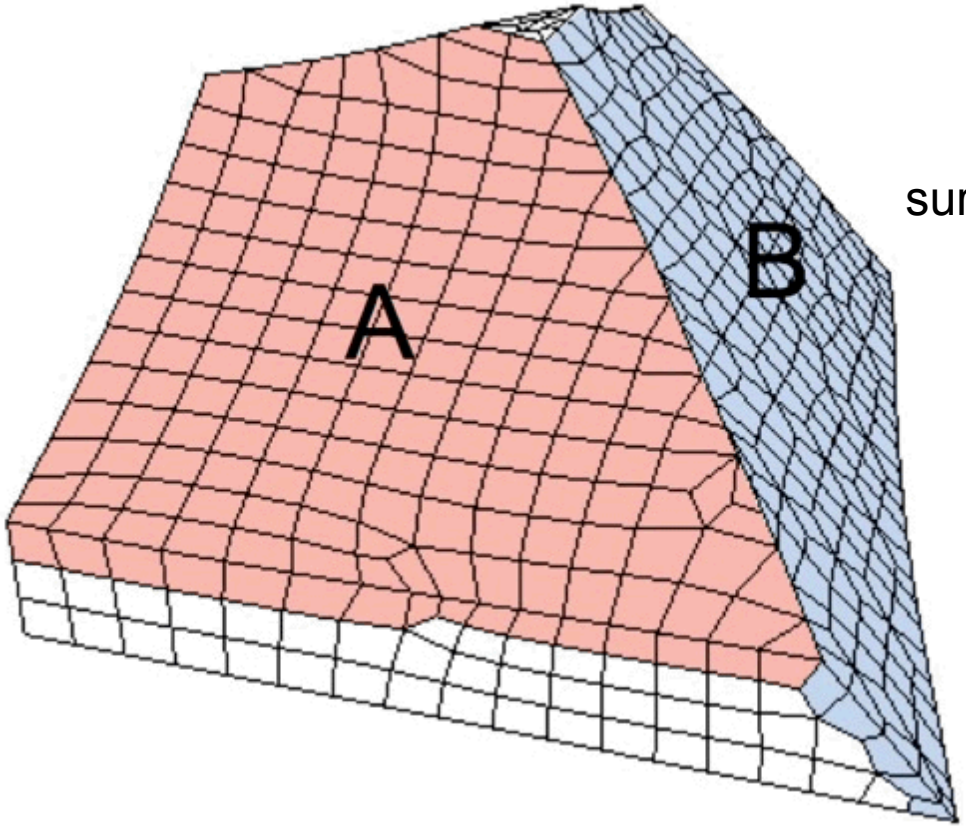


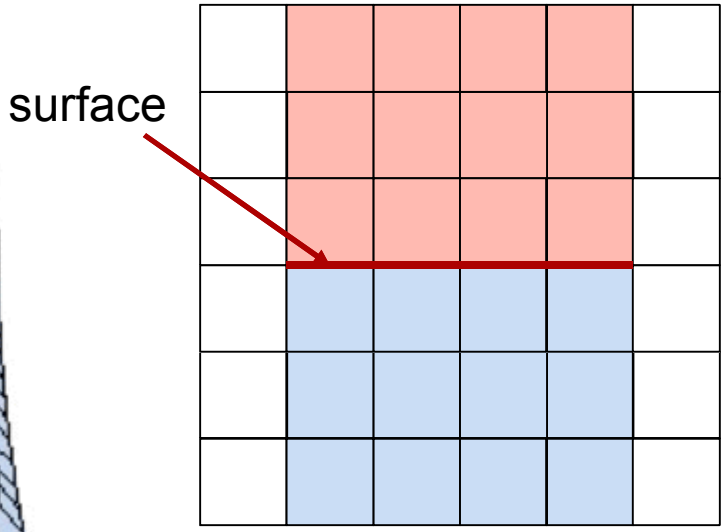


Volume Pillowing

Pillowing







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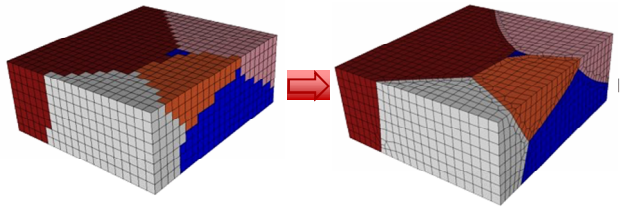
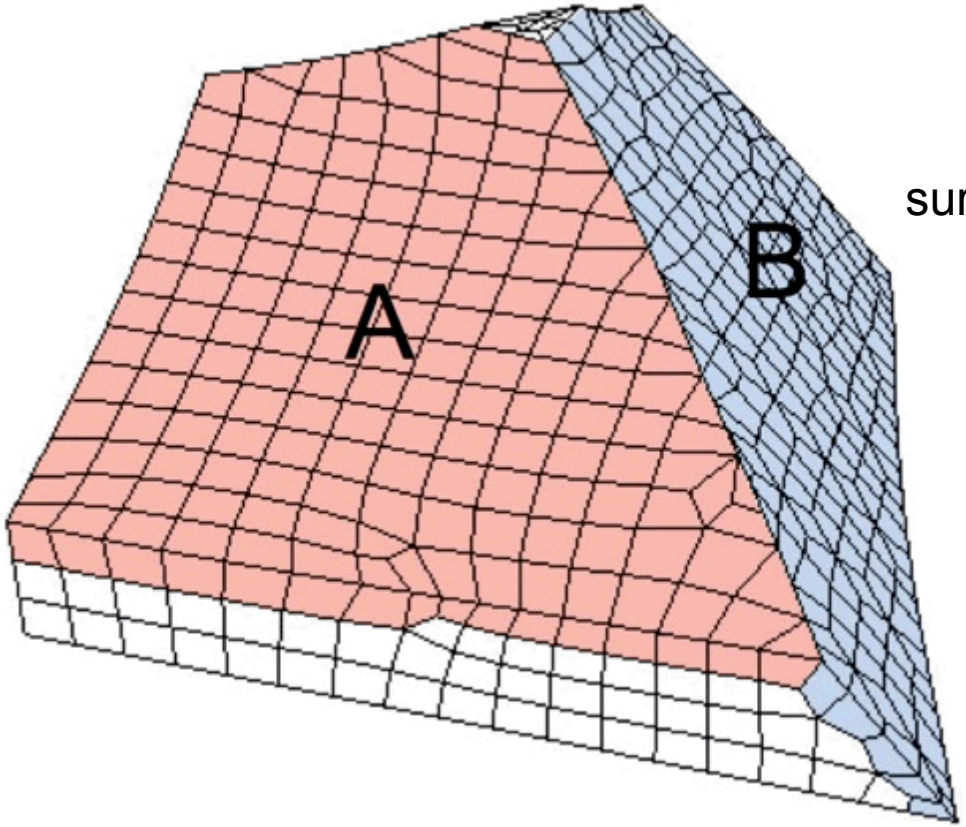
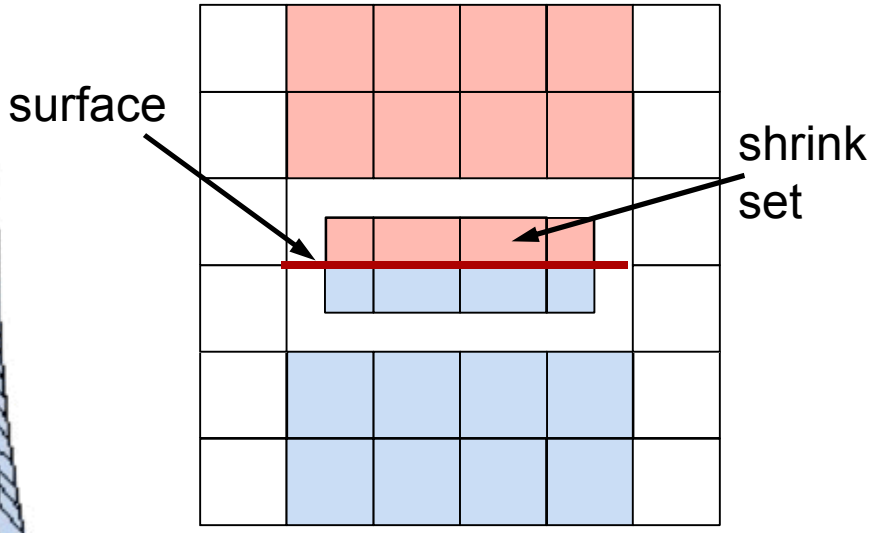
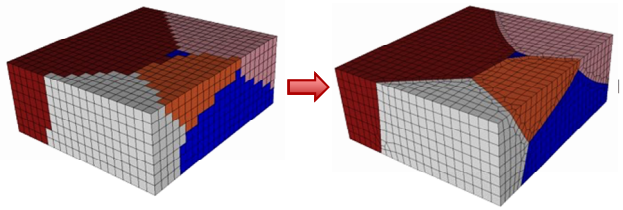


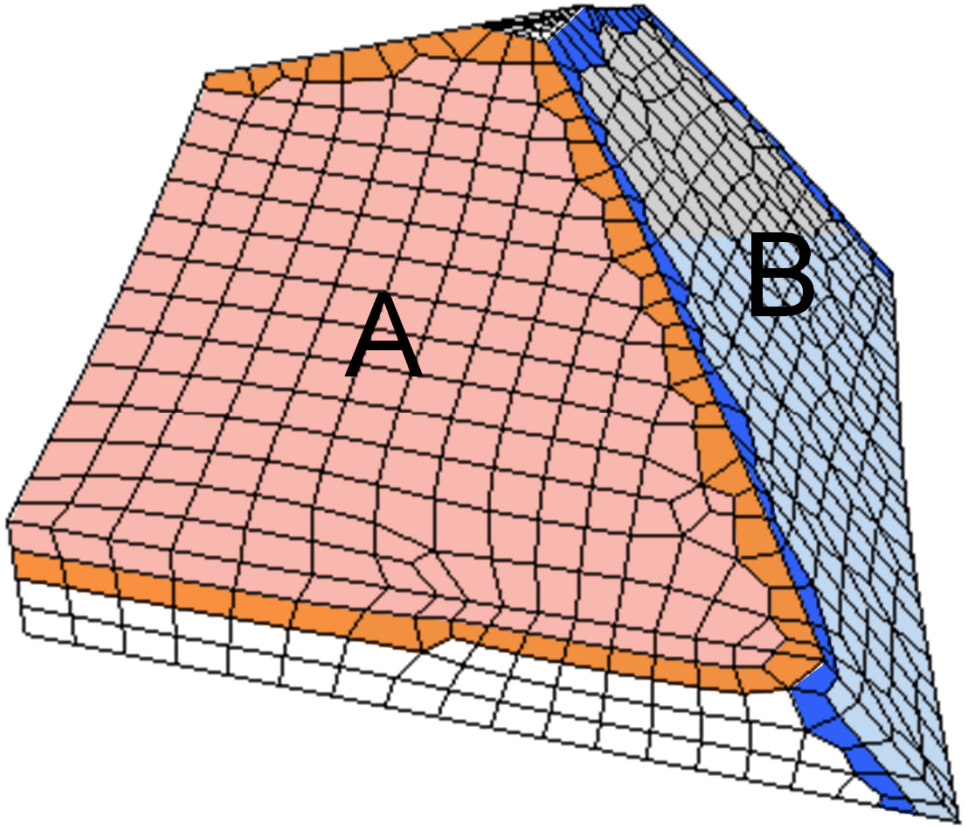


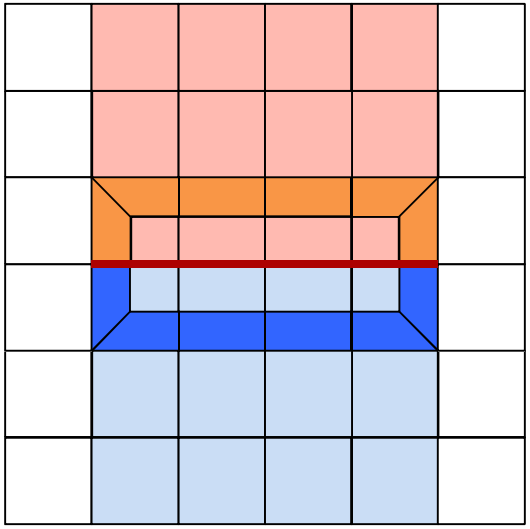


All hexes with a face on a surface are "shrunk"

Pillowing

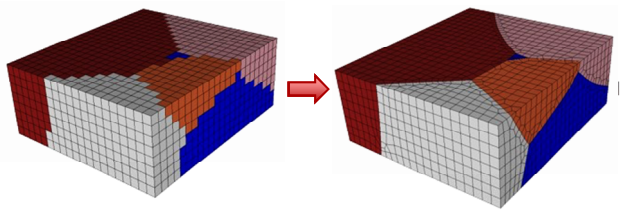


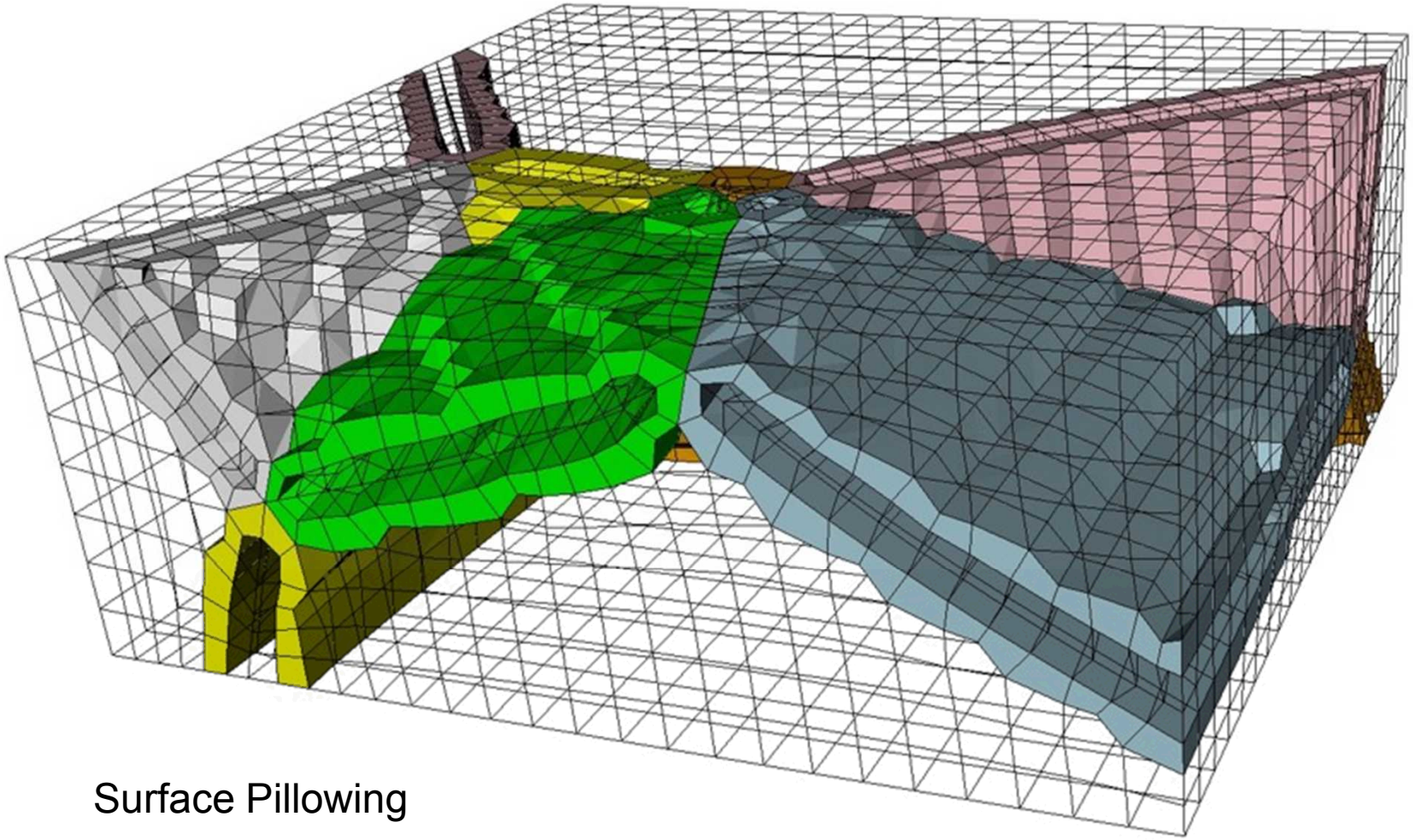




…and a layer of hexes surrounding the shrink set is inserted

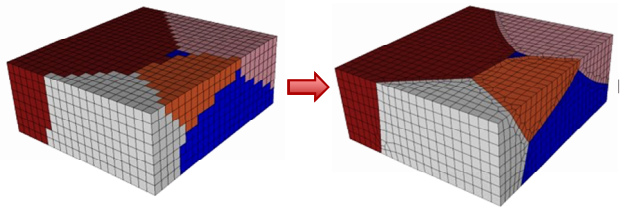
Pillowing

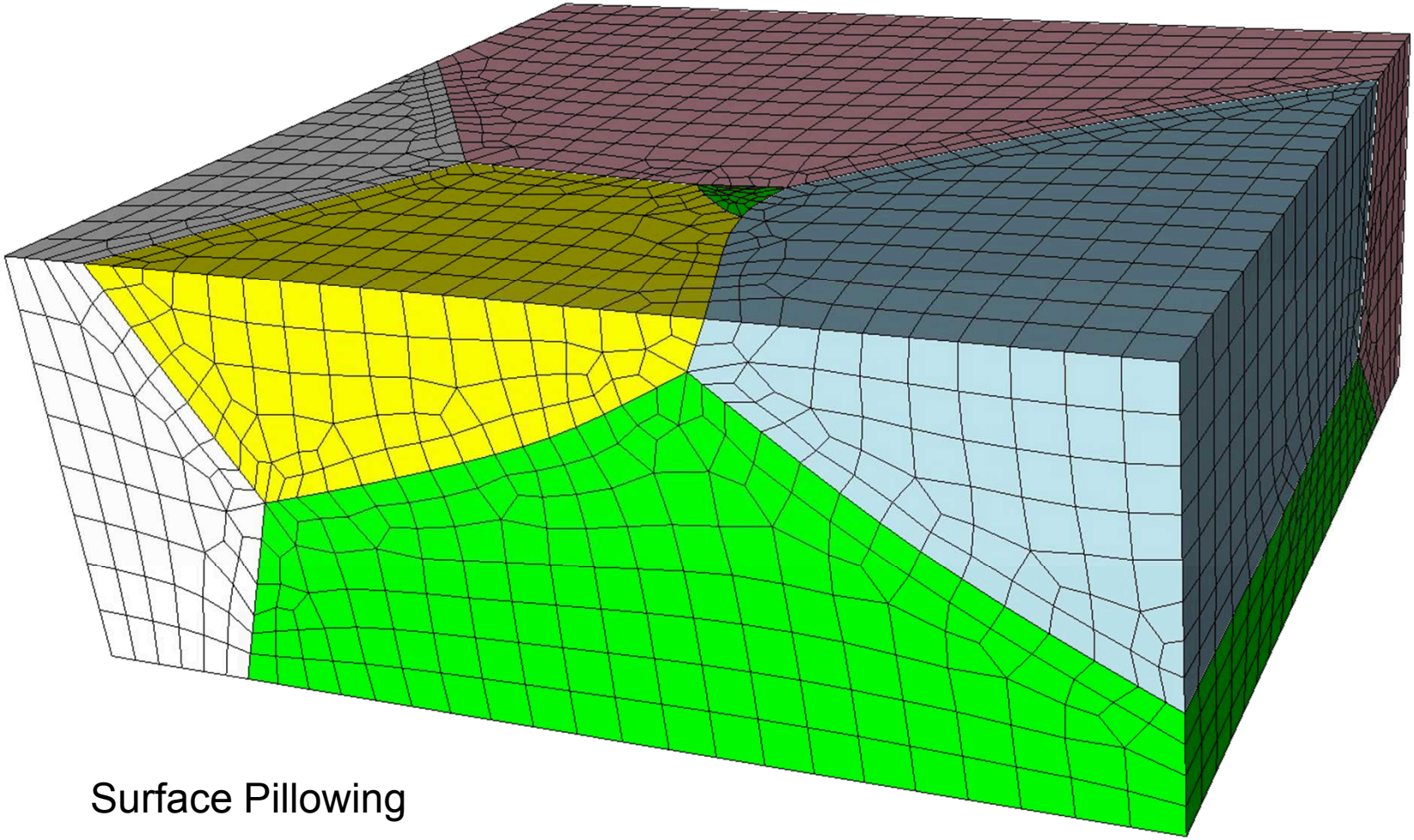




Surface Pillowing

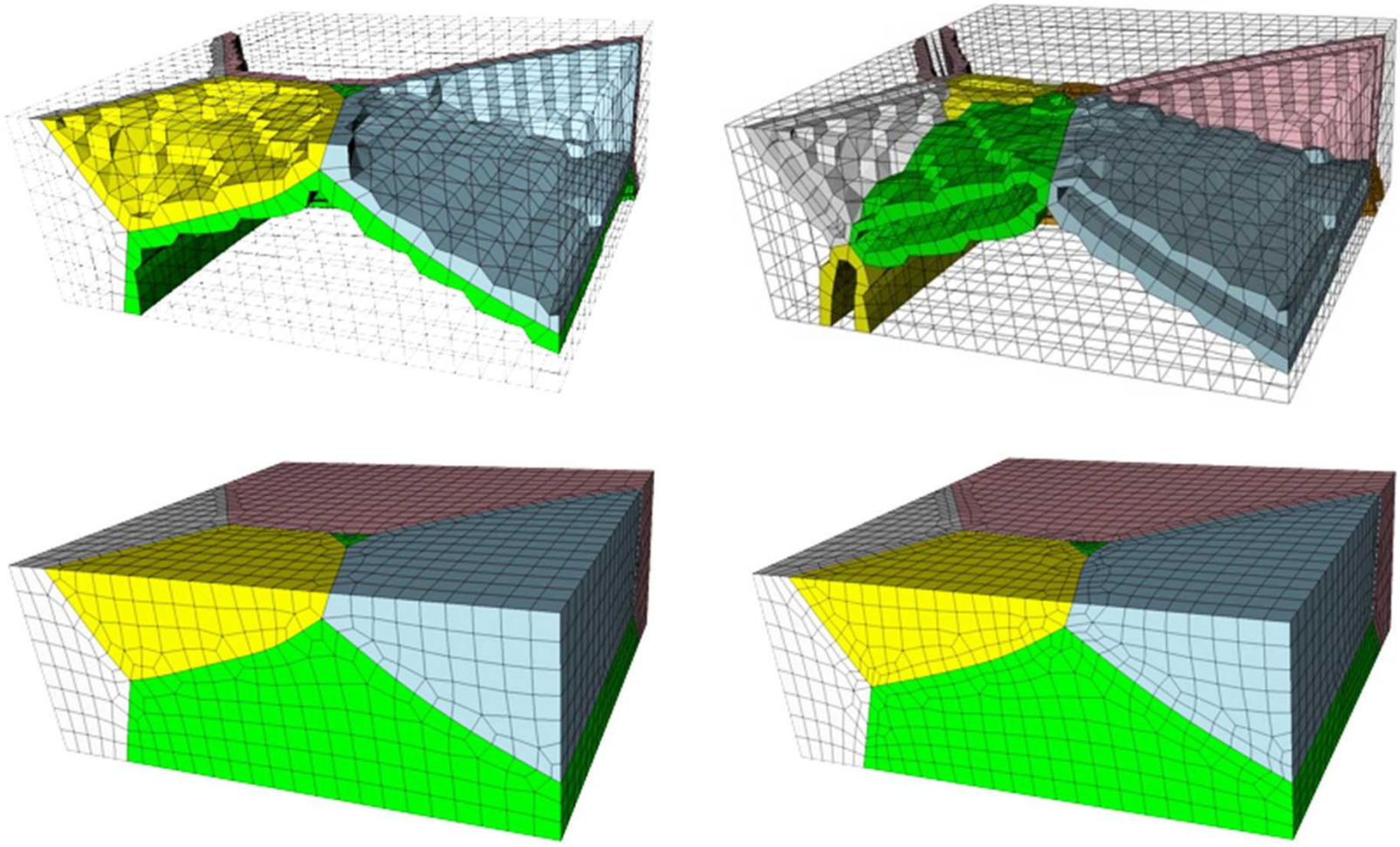
Pillowing





Surface Pillowing

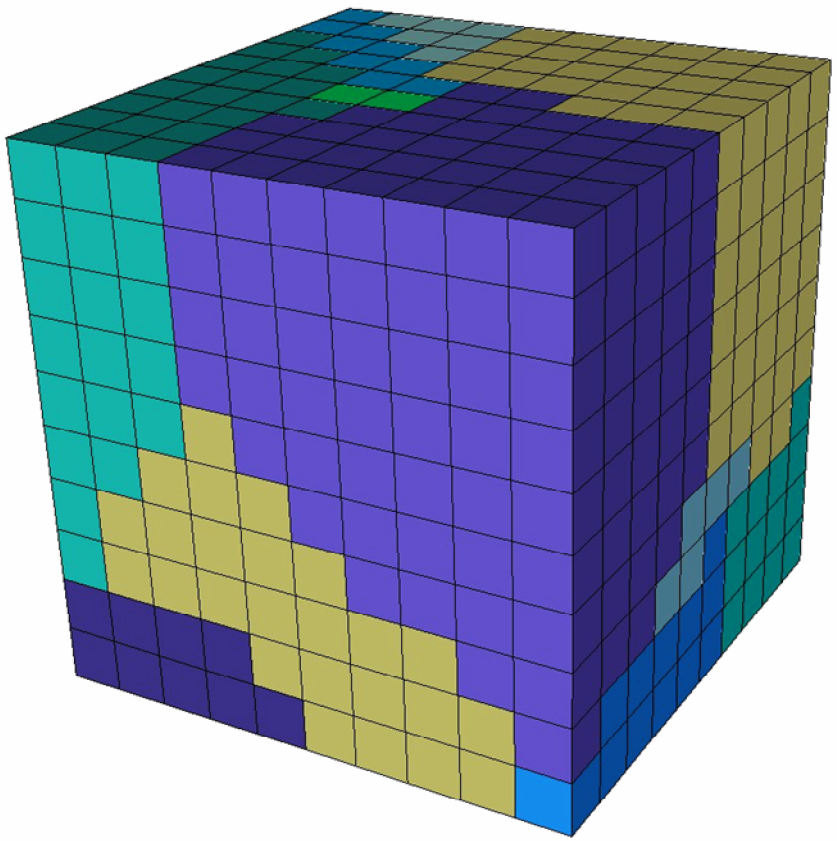
Pillowing

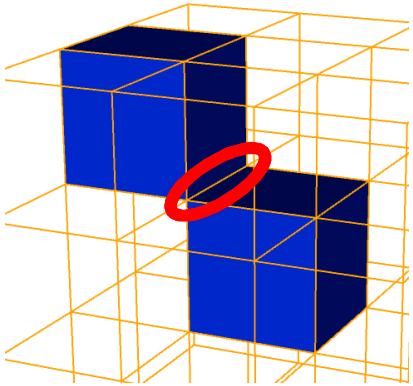


Volume Pillowing

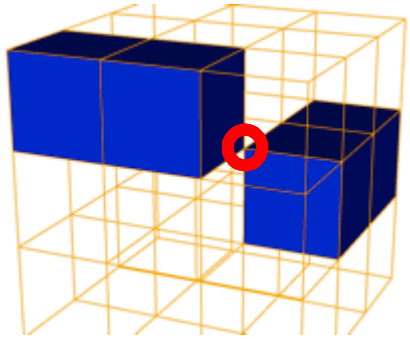
Surface Pillowing

Material Assignment



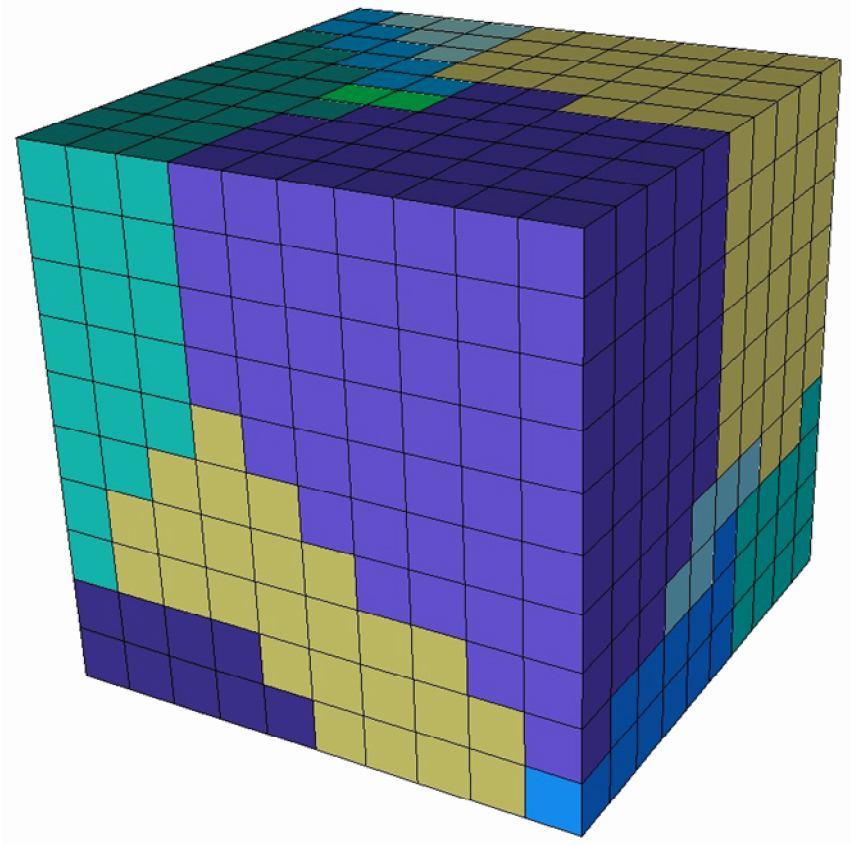


Non-manifold edge

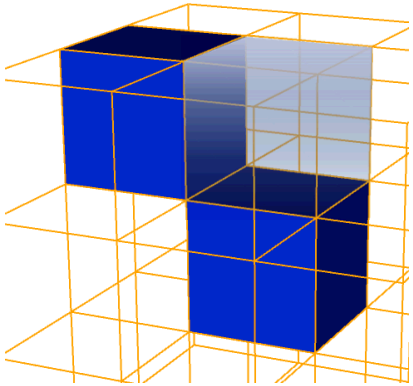


Non-manifold node

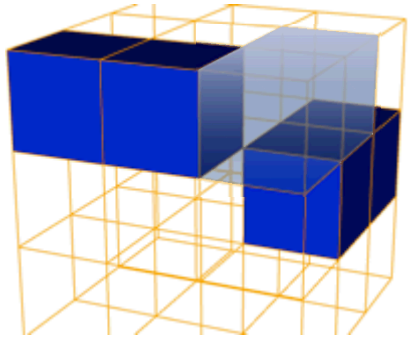
Material Assignment



Non-manifold Resolution

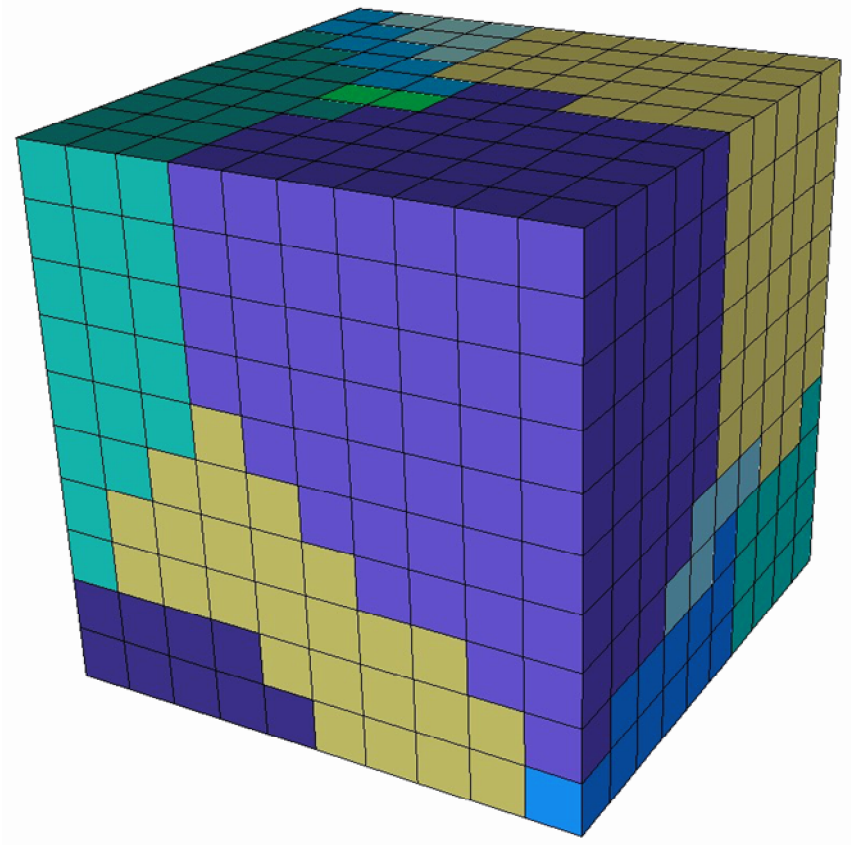


Non-manifold edge

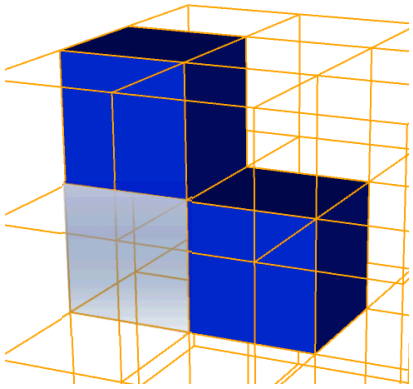


Non-manifold node

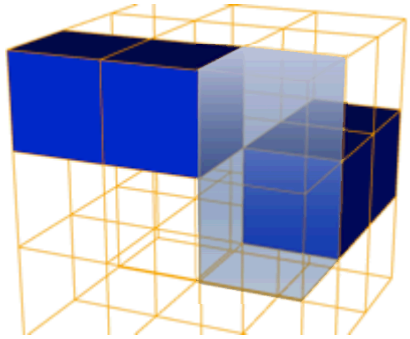
Material Assignment



Non-manifold Resolution

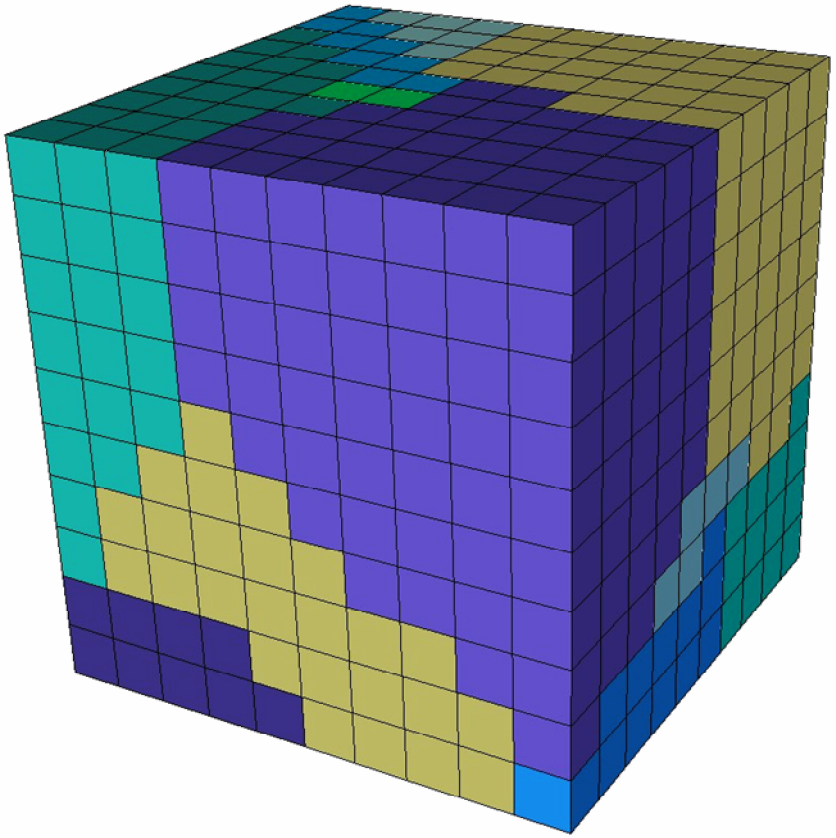


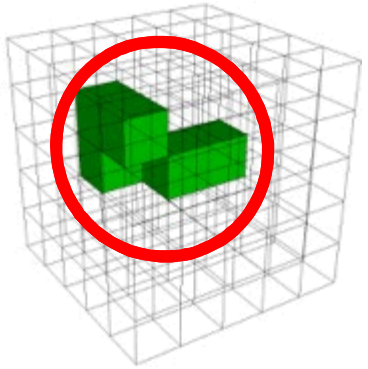
Non-manifold edge



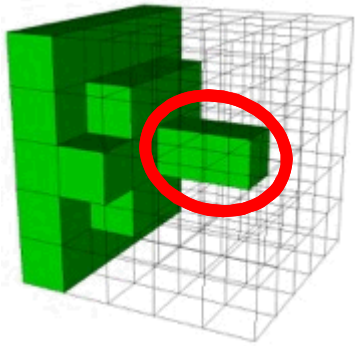
Non-manifold node

Material Assignment

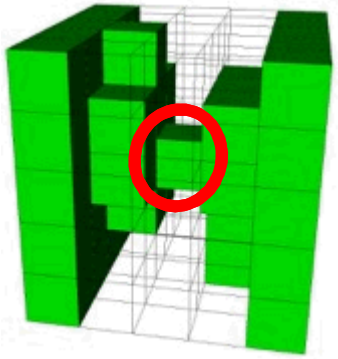




Island

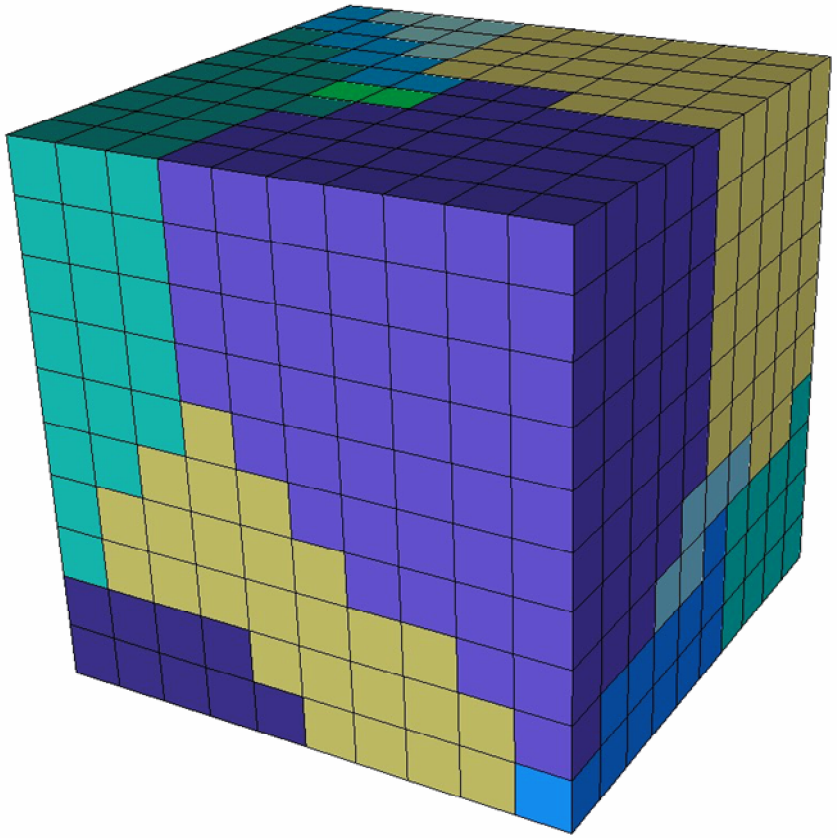


Peninsula

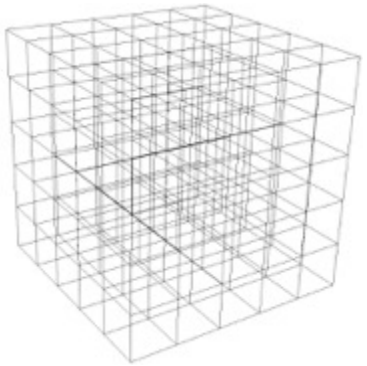


Isthmus

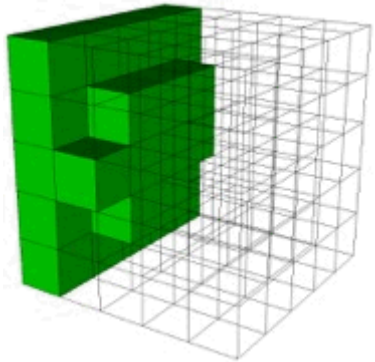
Material Assignment



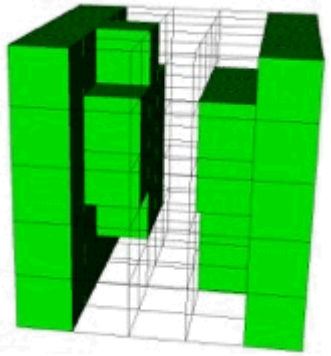
Defeaturing



Island

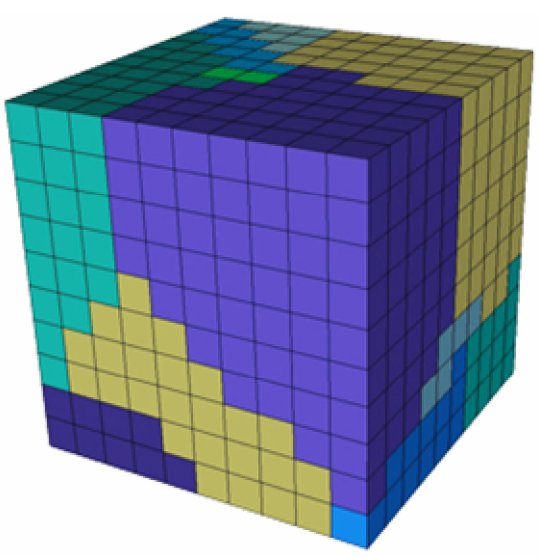


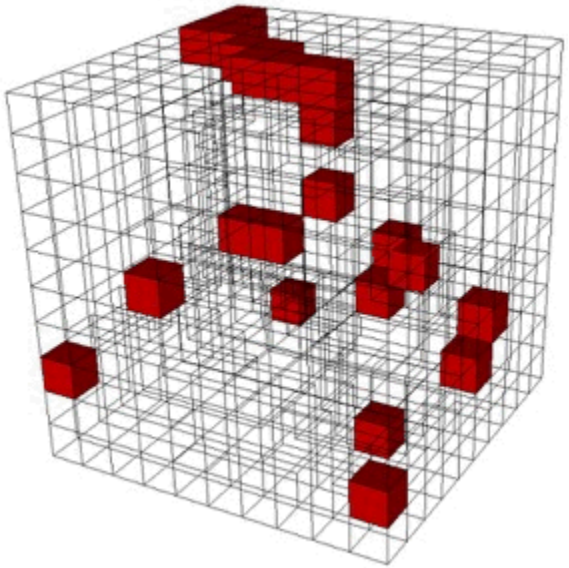
Peninsula

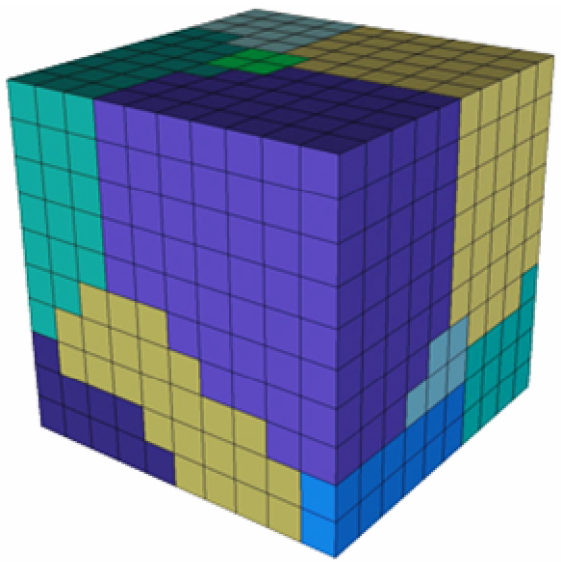


Isthmus

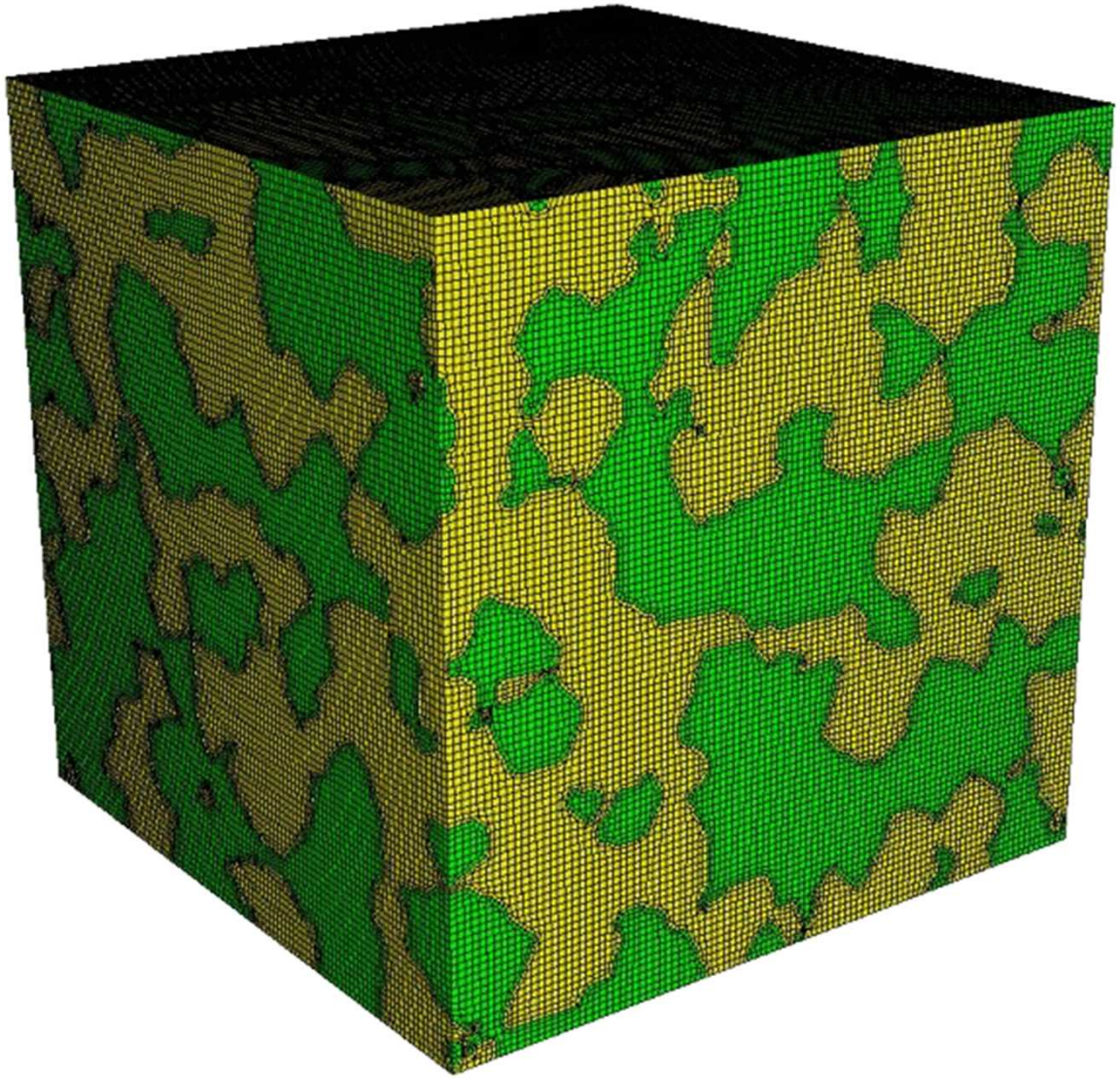
Material Assignment



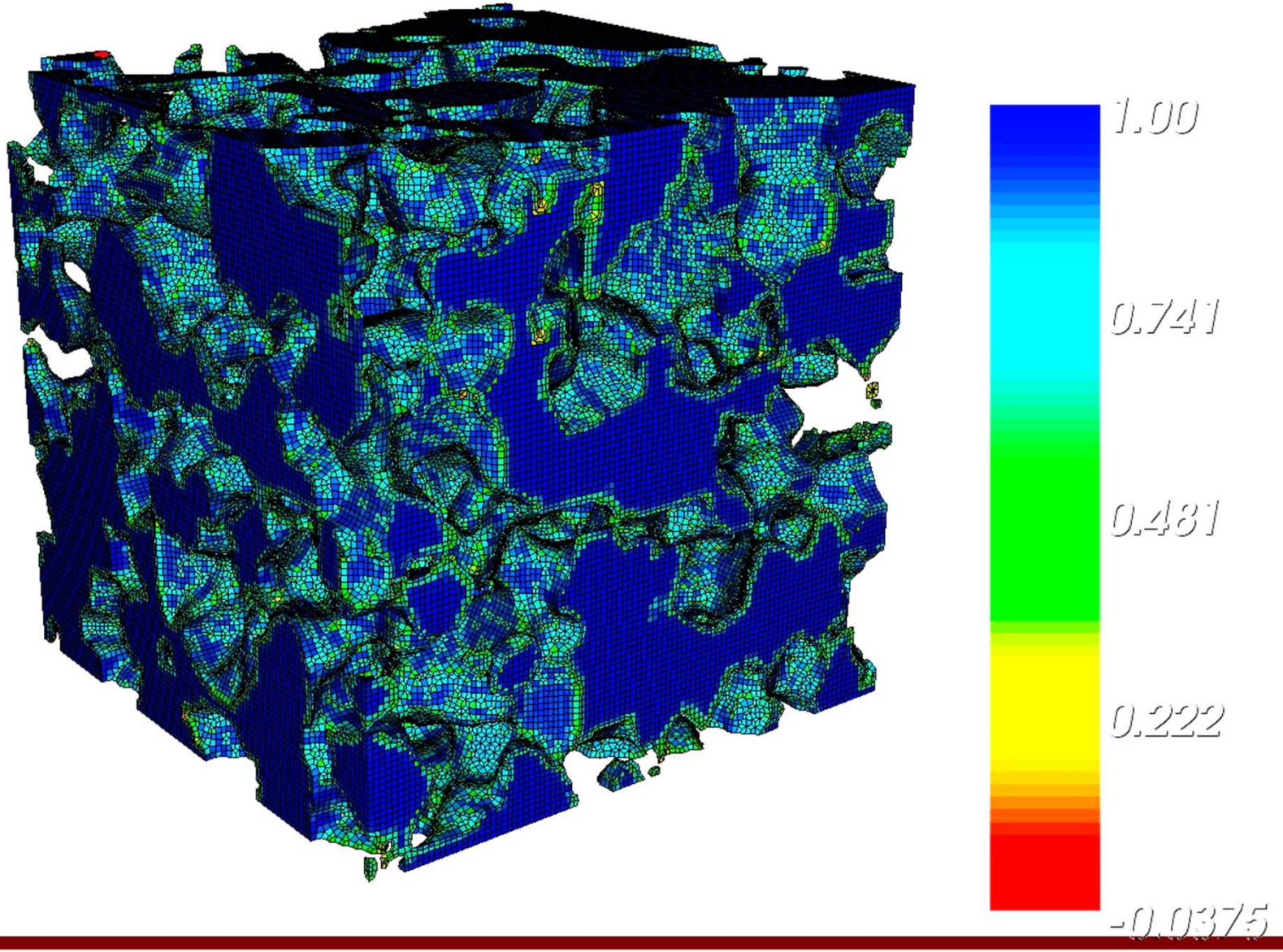




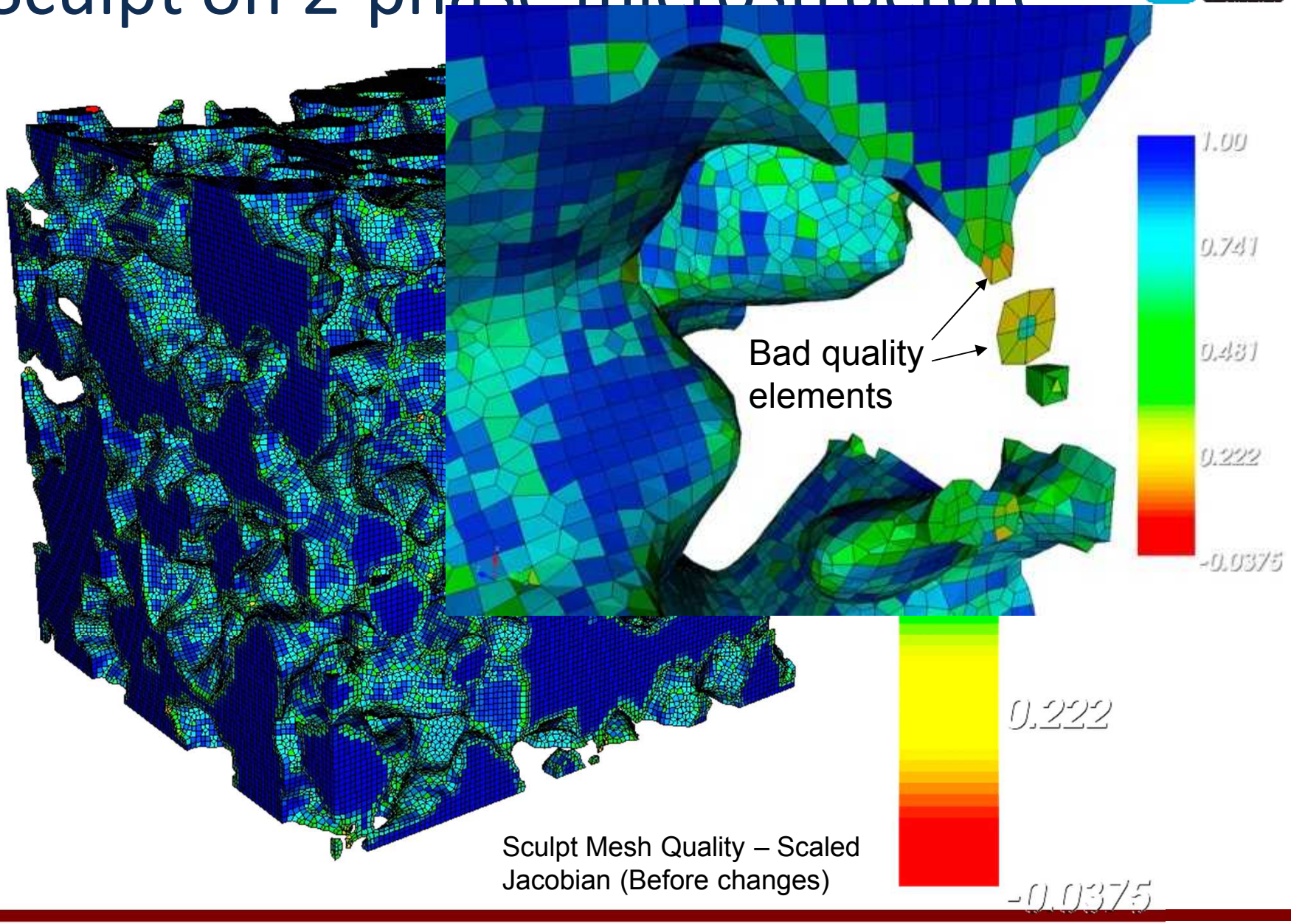
Defeaturing Microstructures



Sculpt on 2-phase microstructure

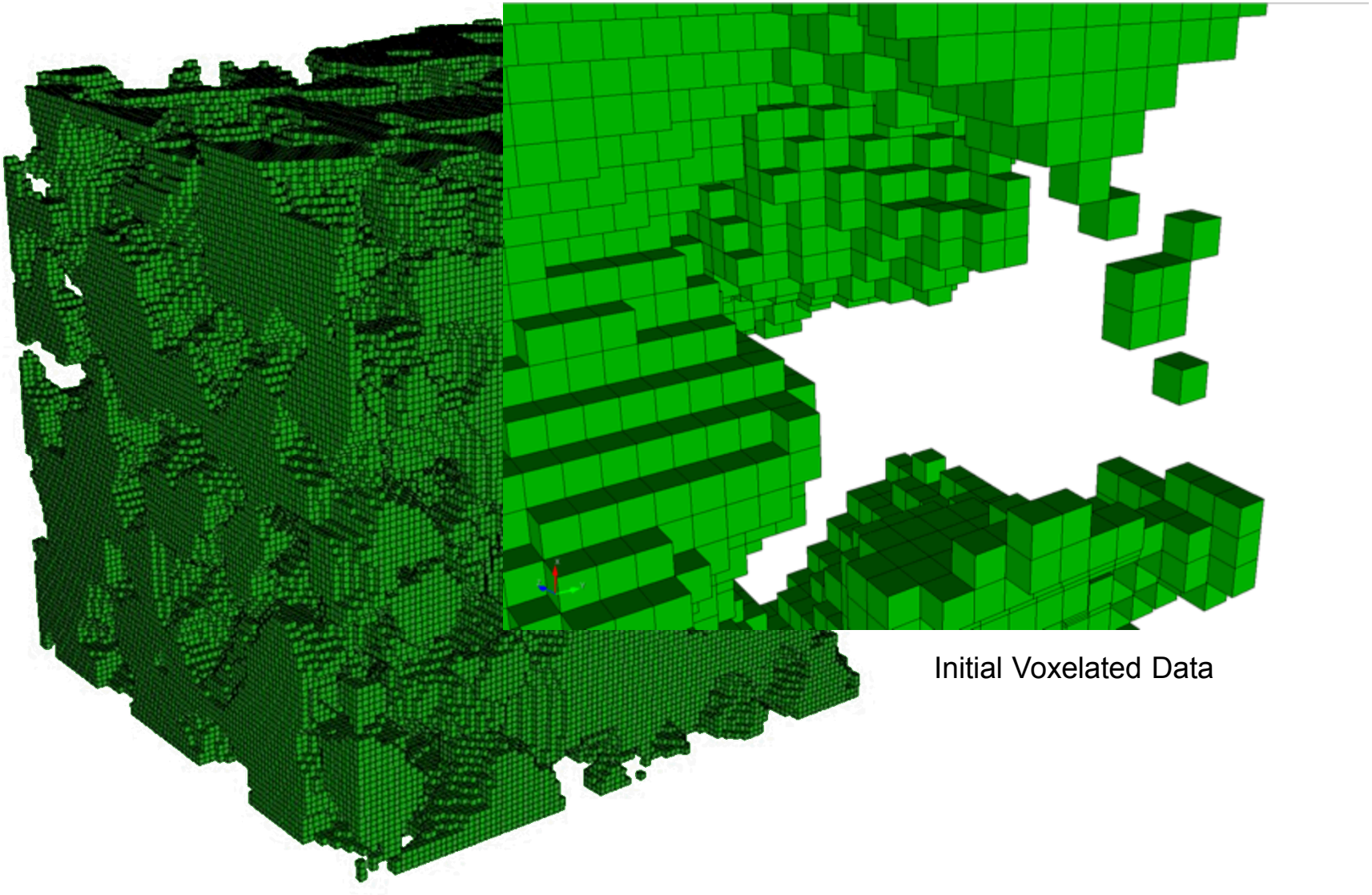


Sculpt on 2-phase microstructure

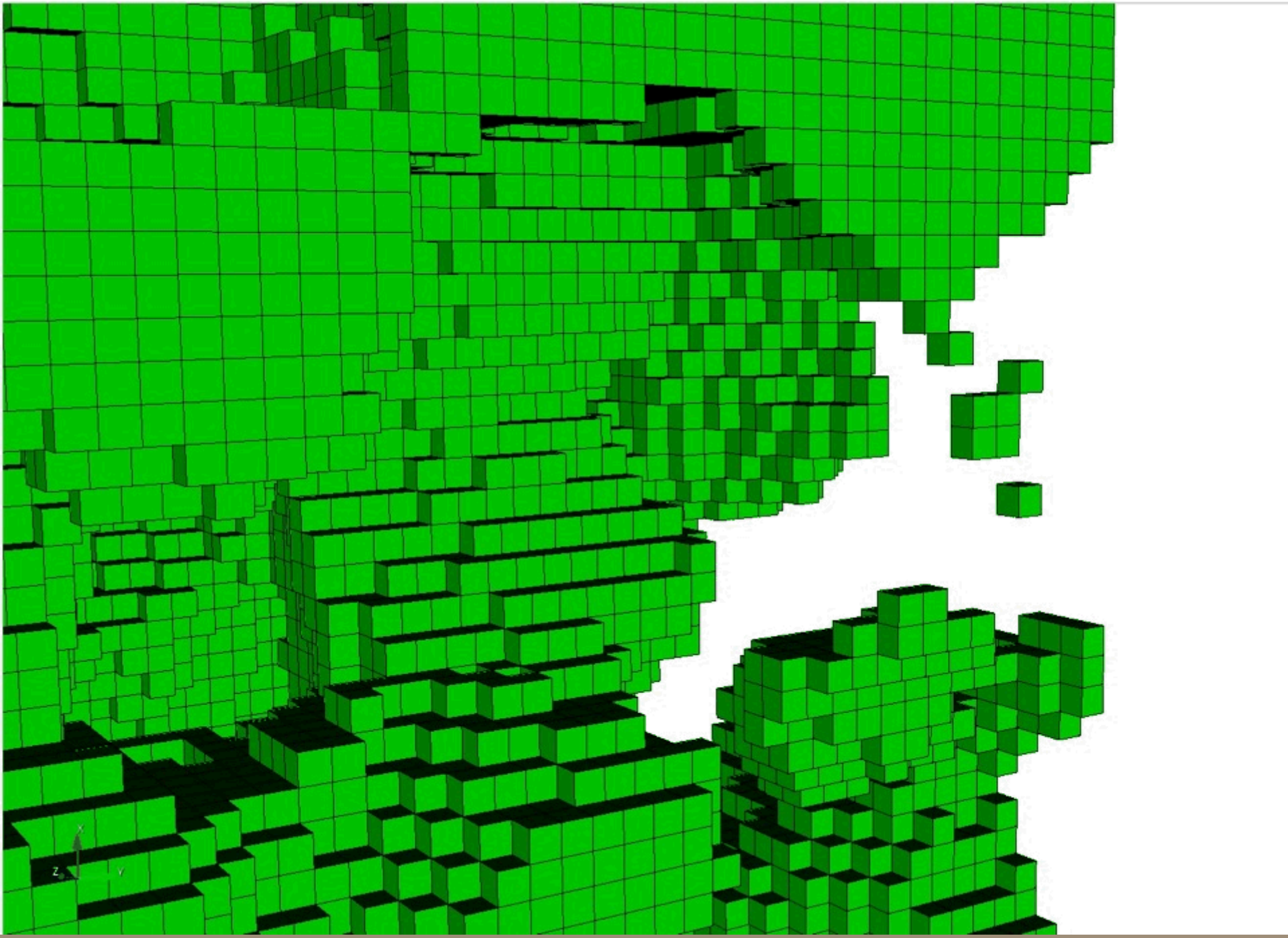


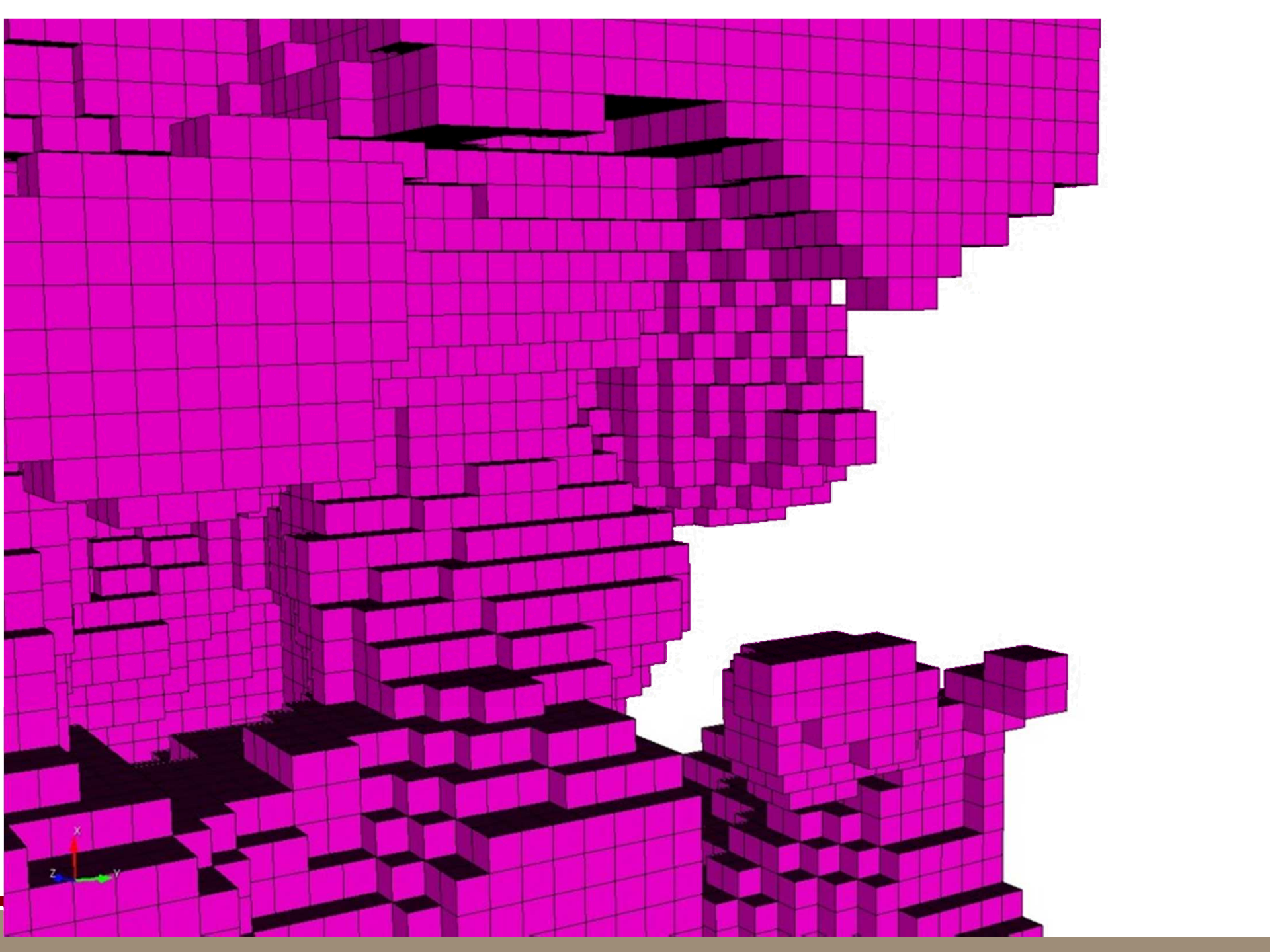
Sculpt Mesh Quality – Scaled Jacobian (Before changes)

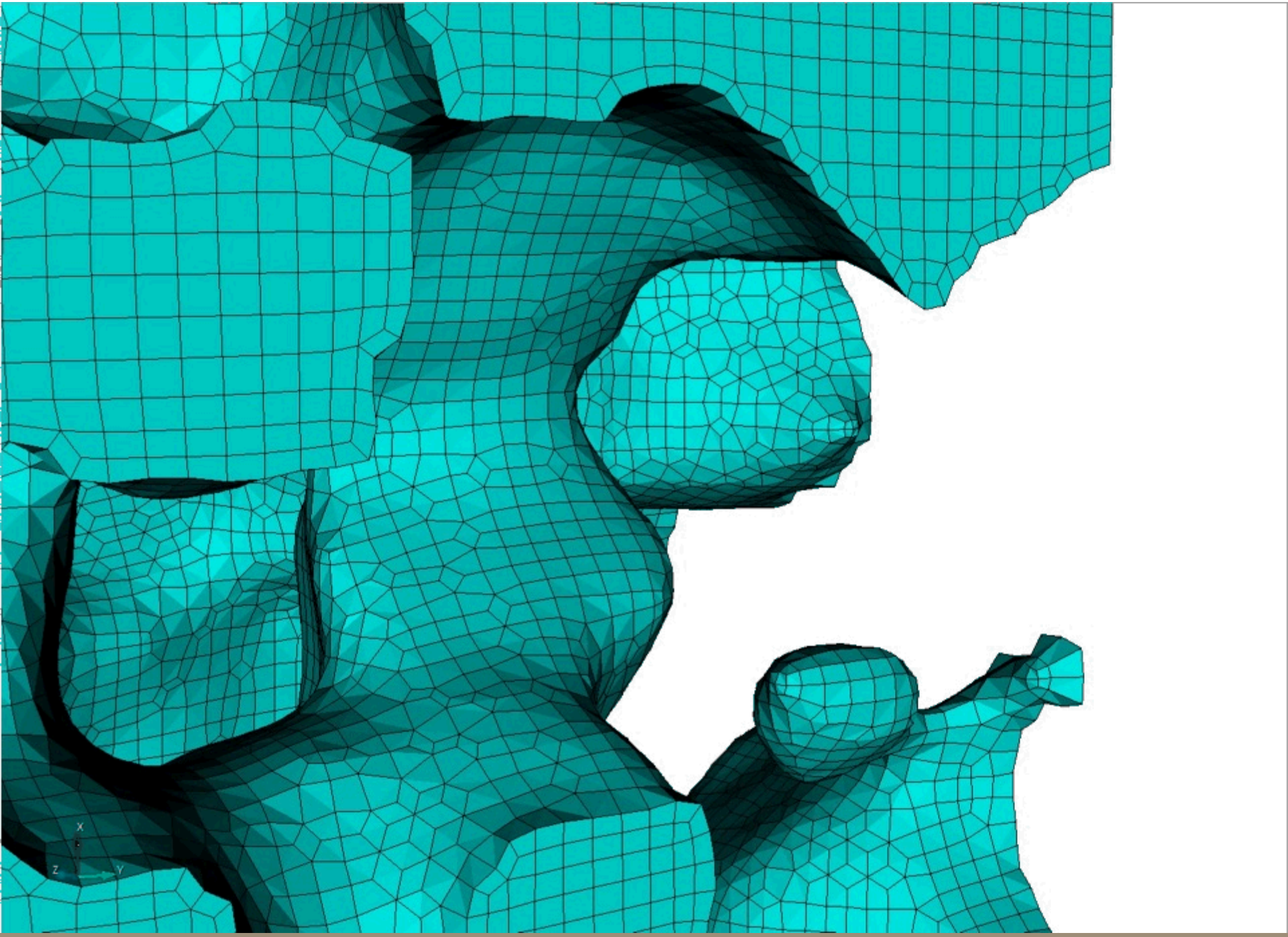
Sculpt on 2-phase microstructure

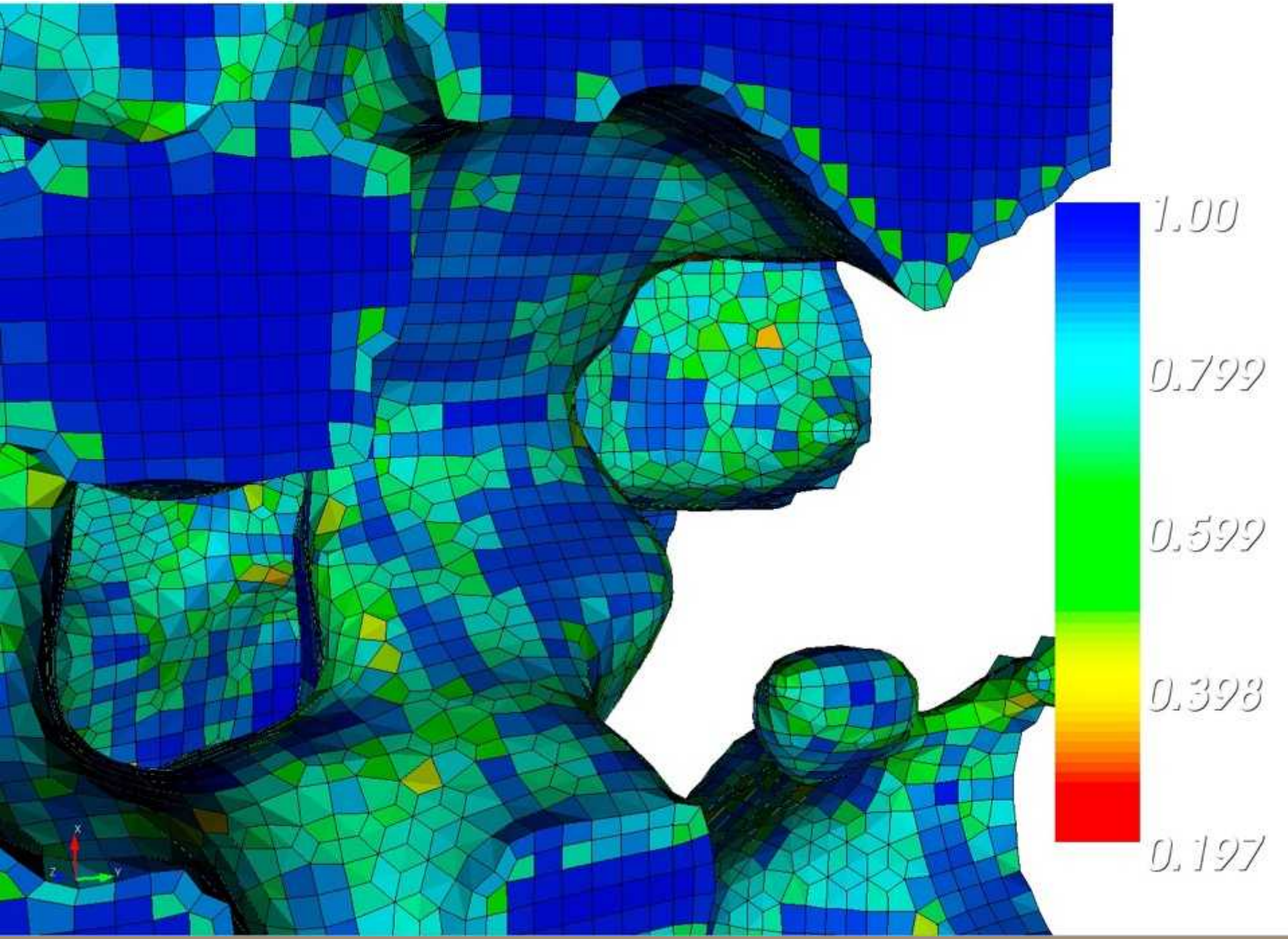


Initial Voxelated Data

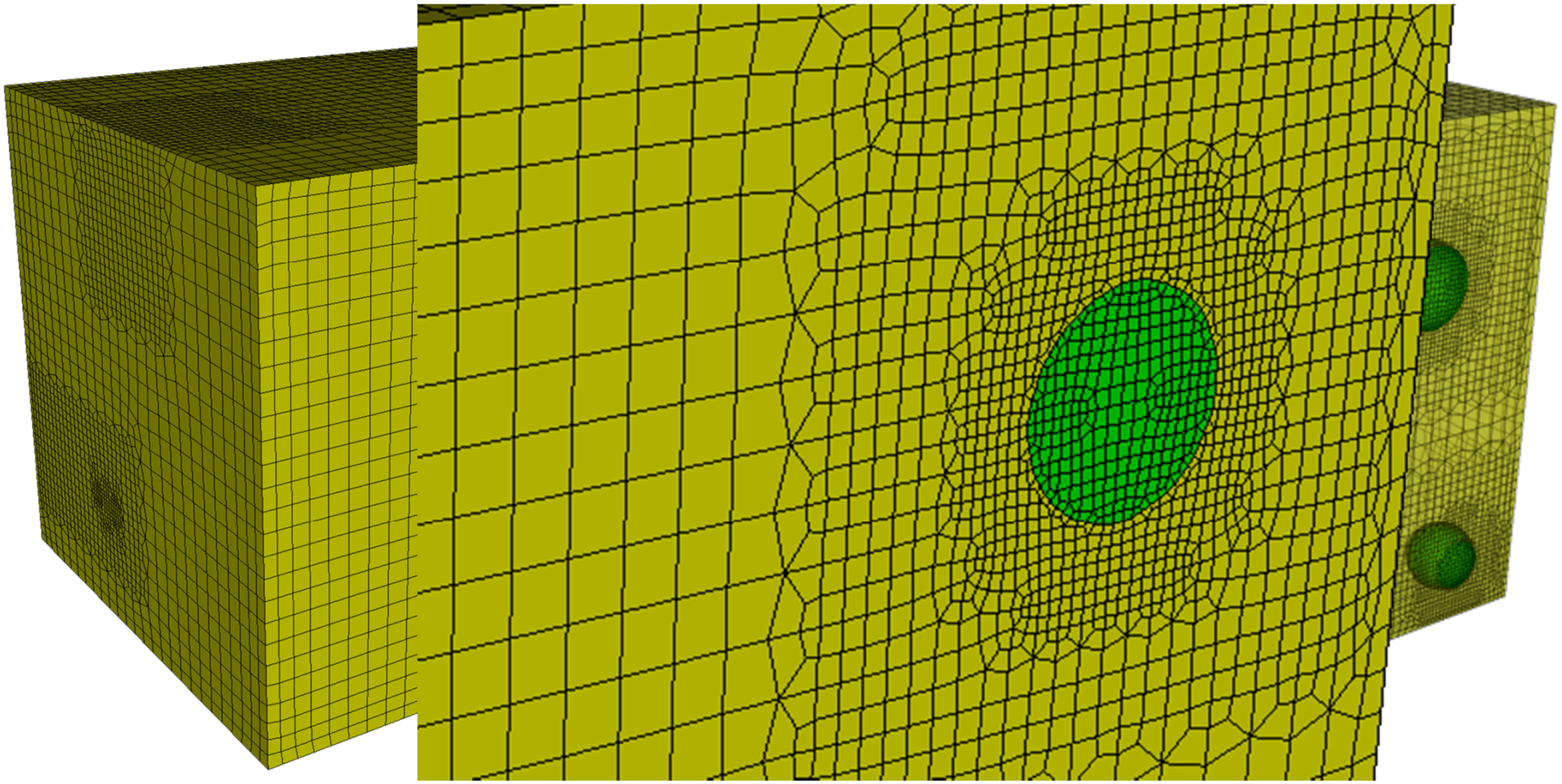



X
Z
Y


X
Z
Y

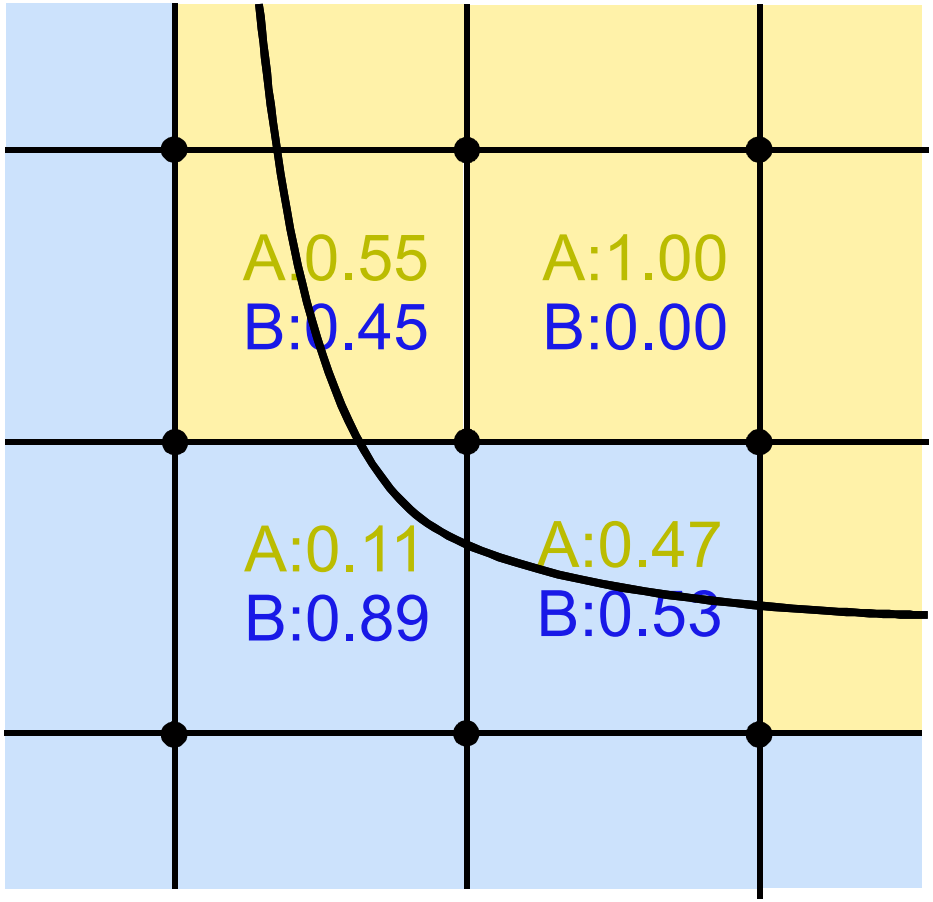

1.00
0.799
0.599
0.398
0.197
X
Z
Y

Adaptive Hex

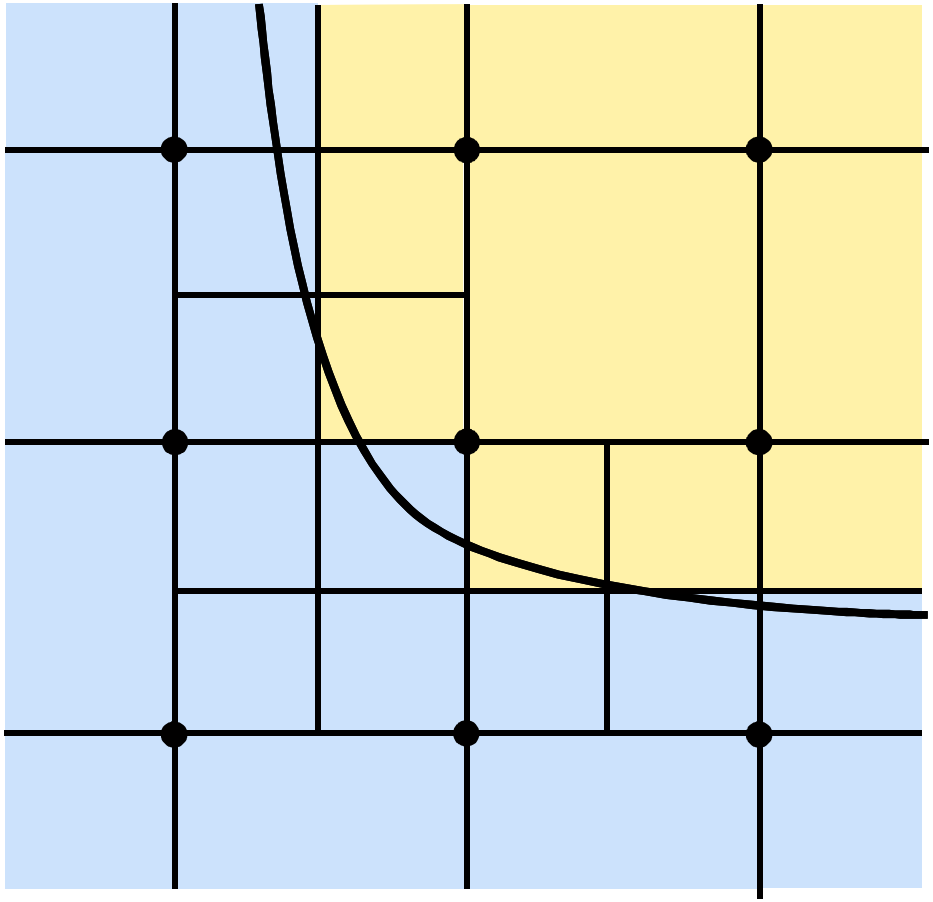


Base Cartesian grid is automatically refined to resolve geometric feaures

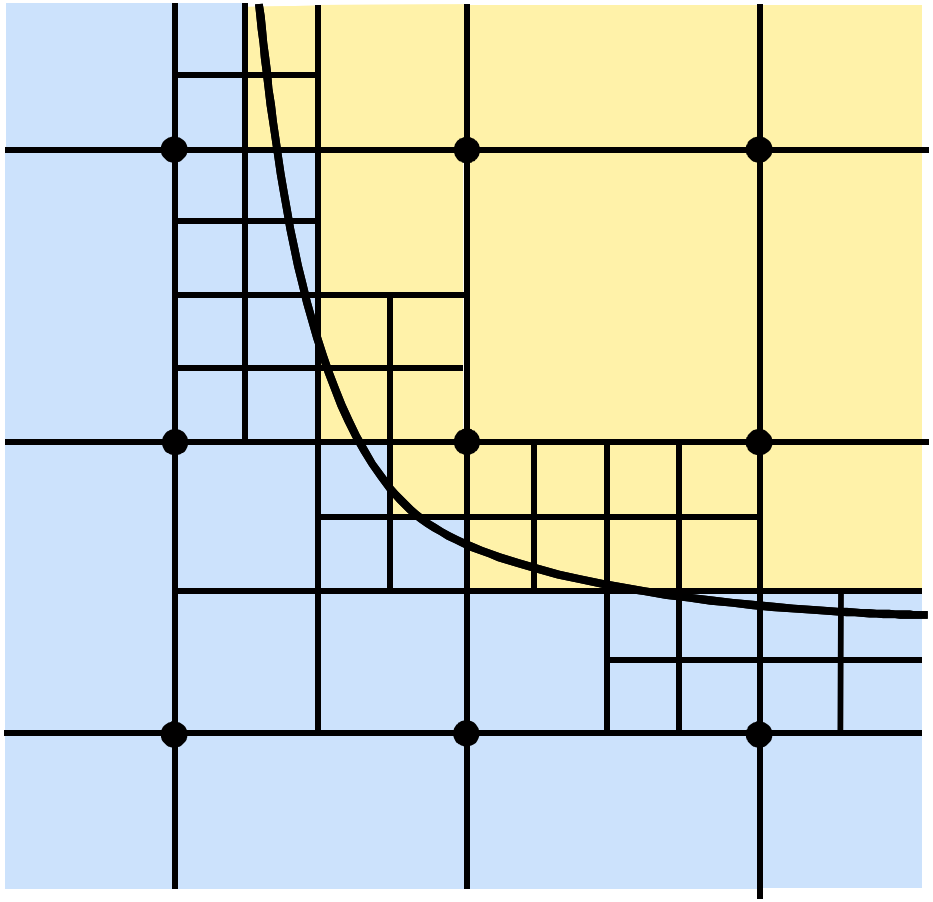
Adaptive Hex



Adaptive Hex



Adaptive Hex



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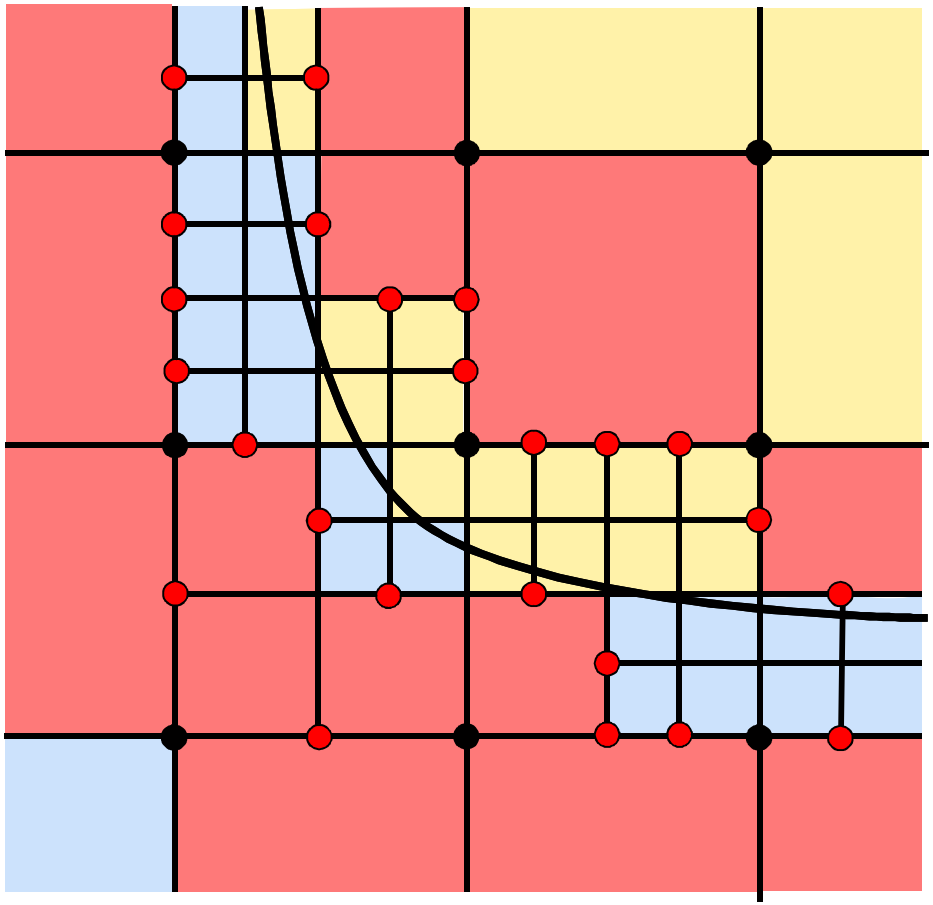
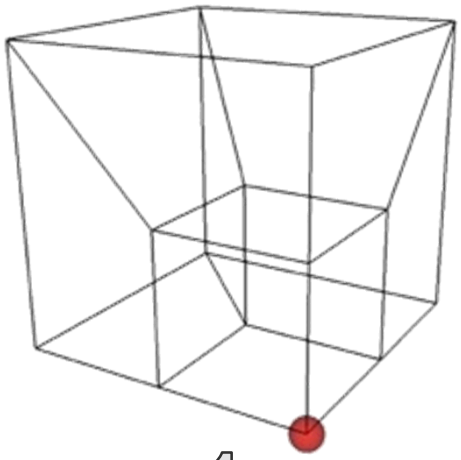
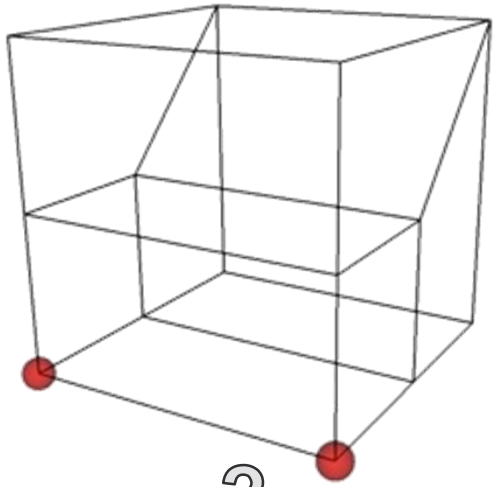


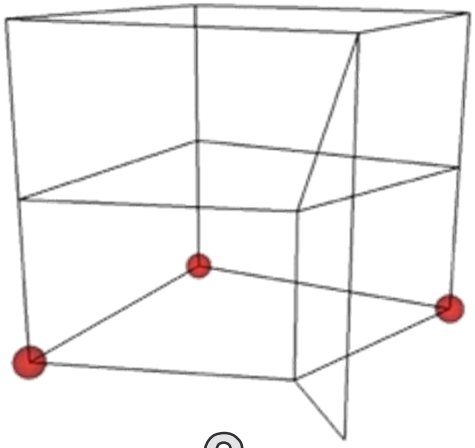
Adaptive Hex



1



2



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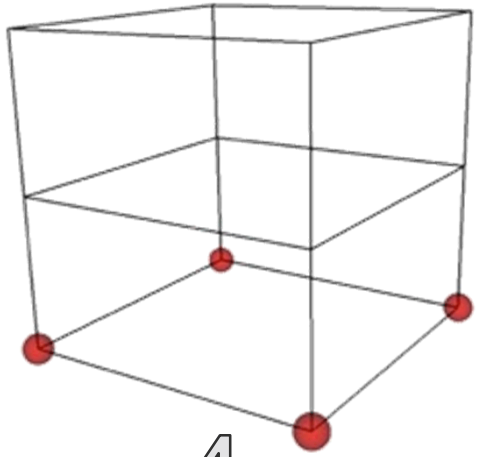
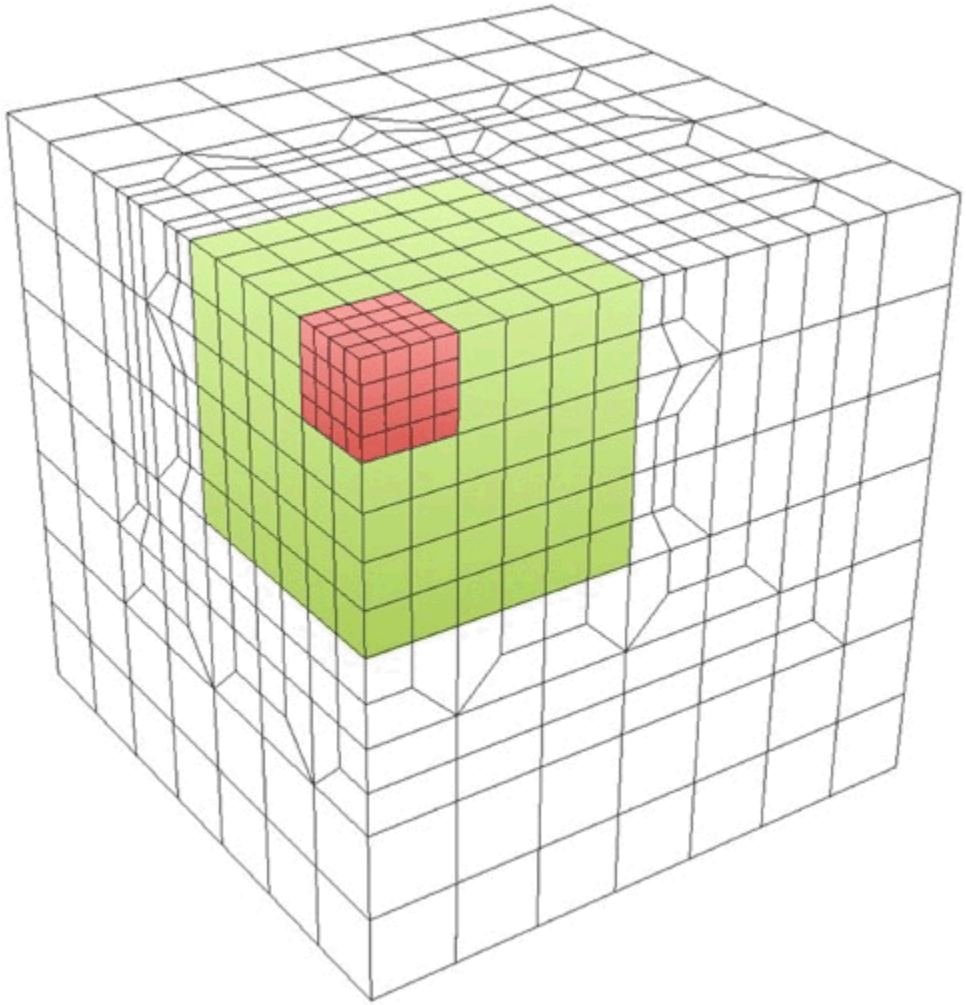
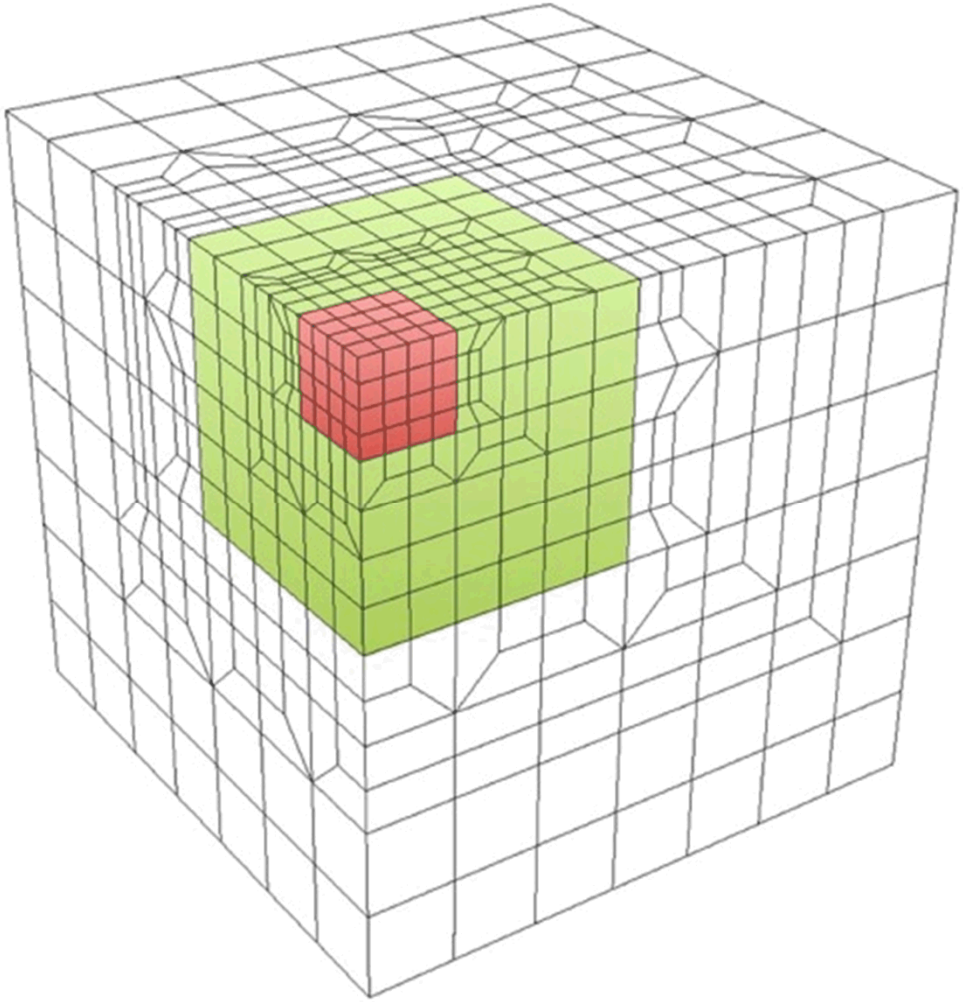


4

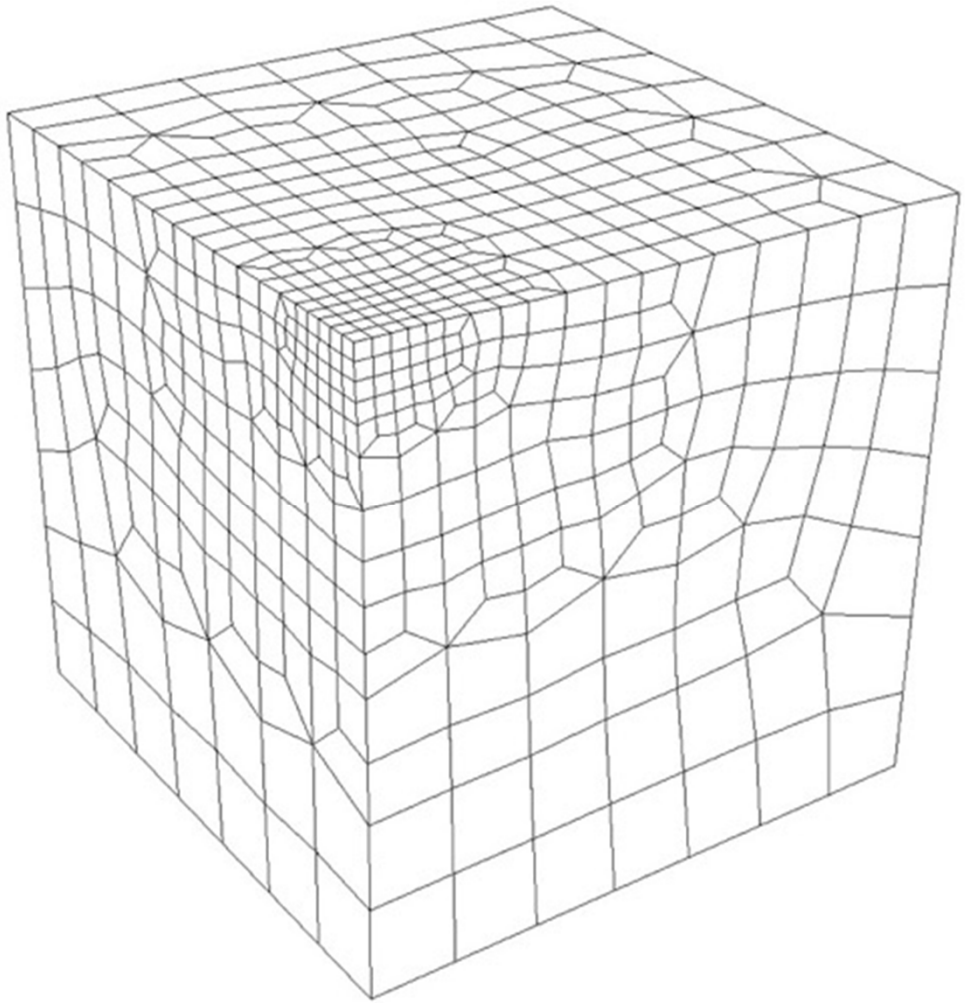
Adaptive Hex



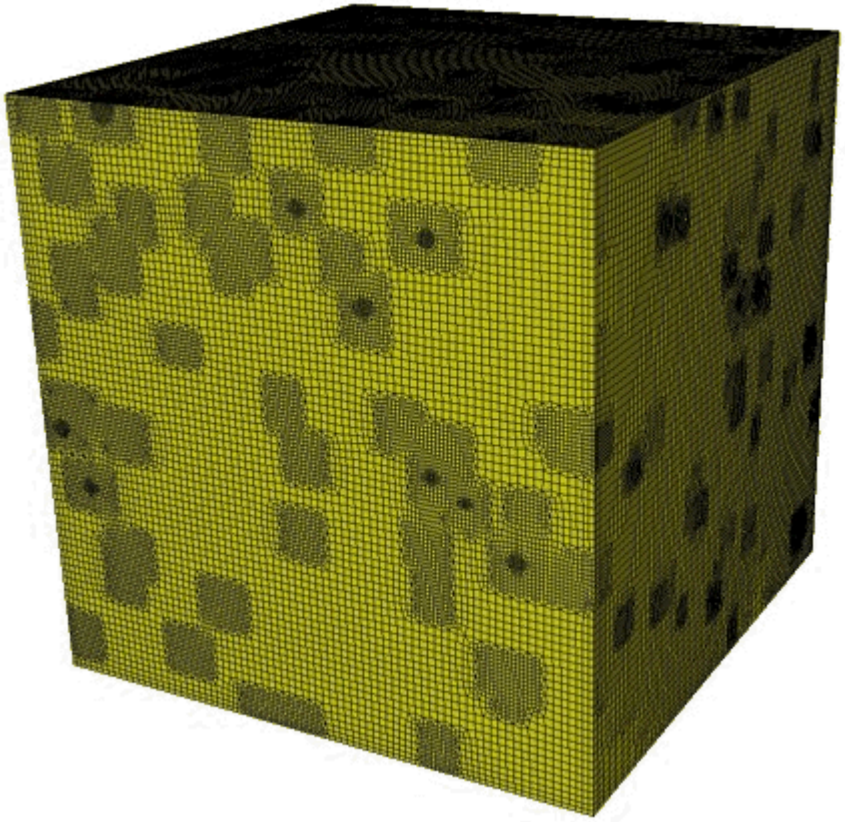
Adaptive Hex



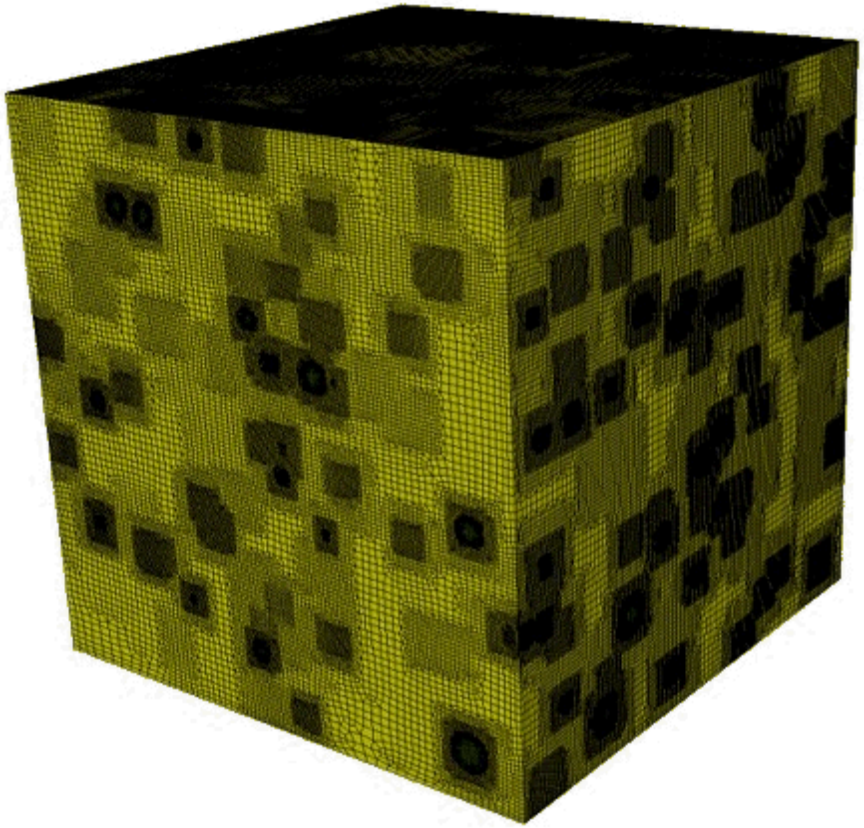
Adaptive Hex



Adaptive Hex

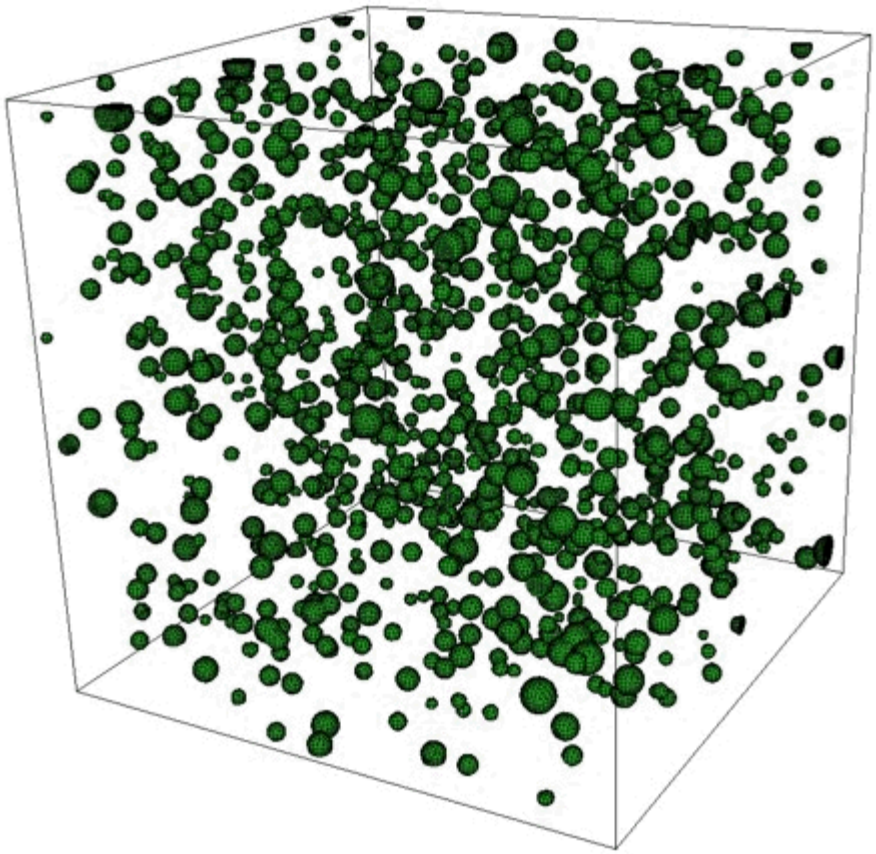


2 Refinement Levels
2,289,900 Hexes

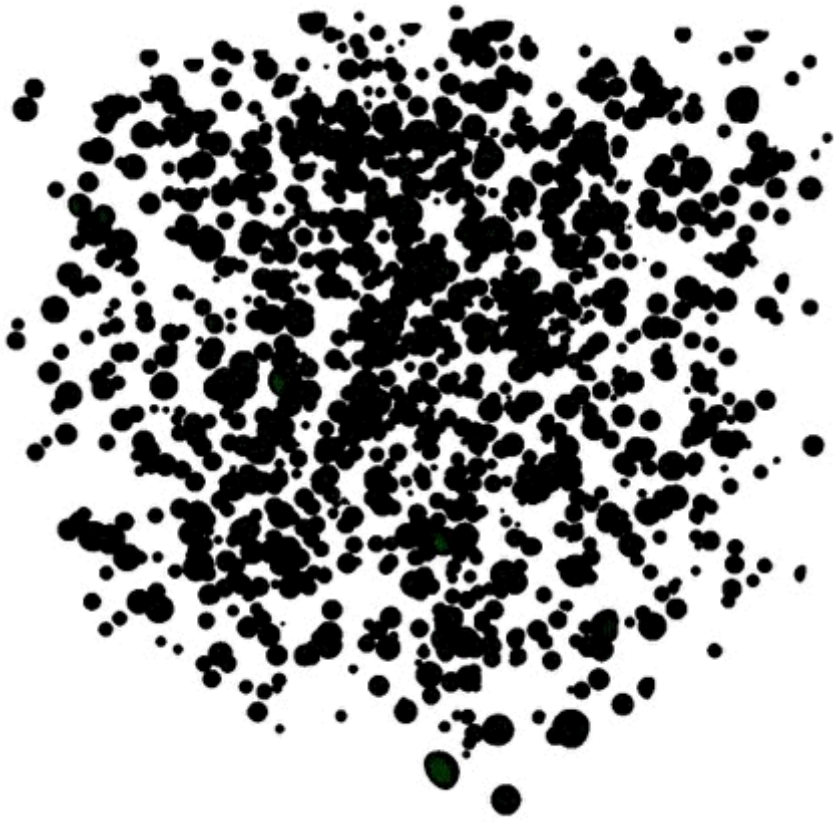


4 Refinement Levels
35,336,356 Hexes

Adaptive Hex

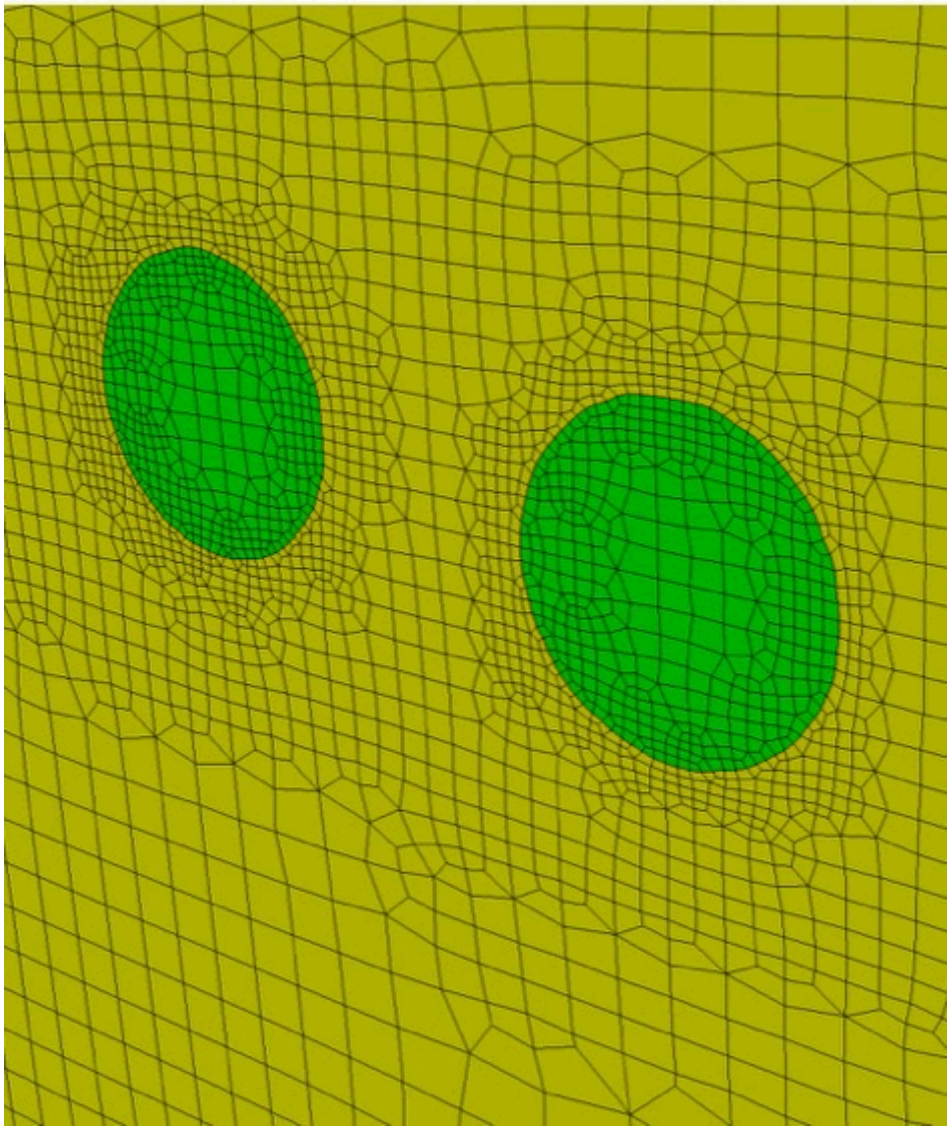


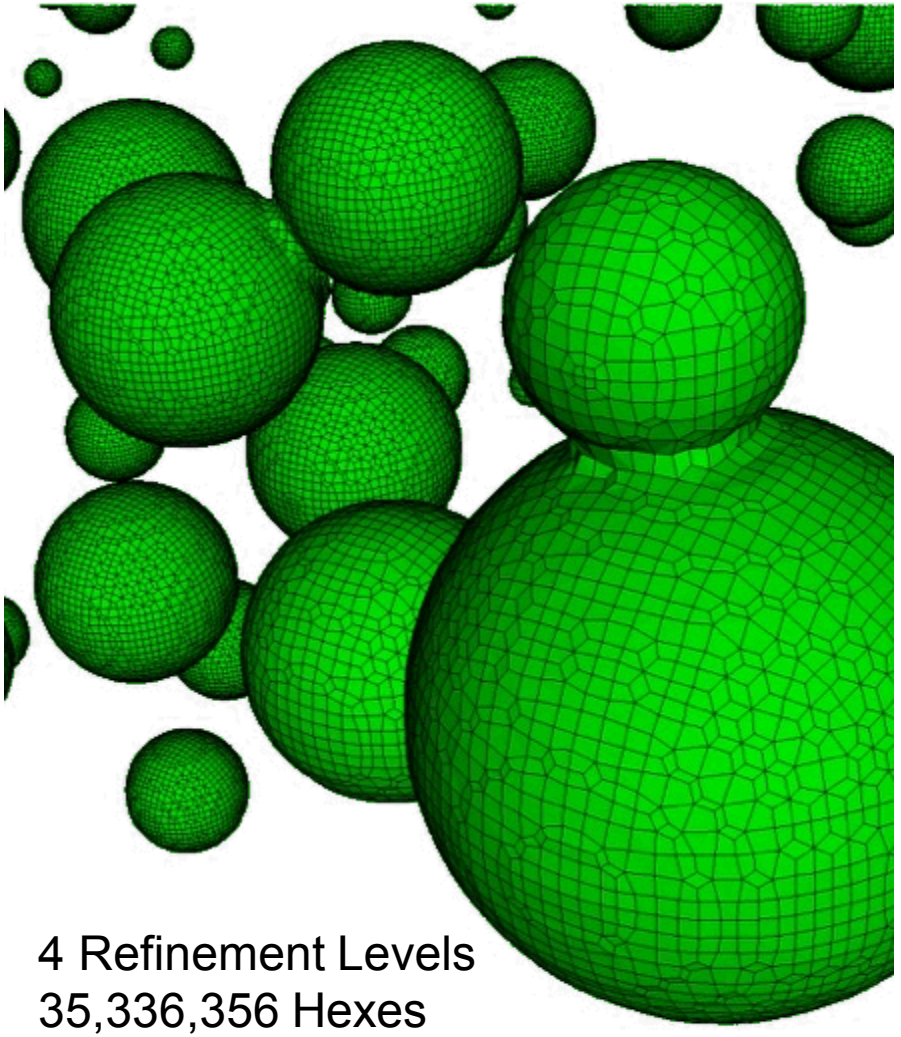
2 Refinement Levels
2,289,900 Hexes



4 Refinement Levels
35,336,356 Hexes

Adaptive Hex

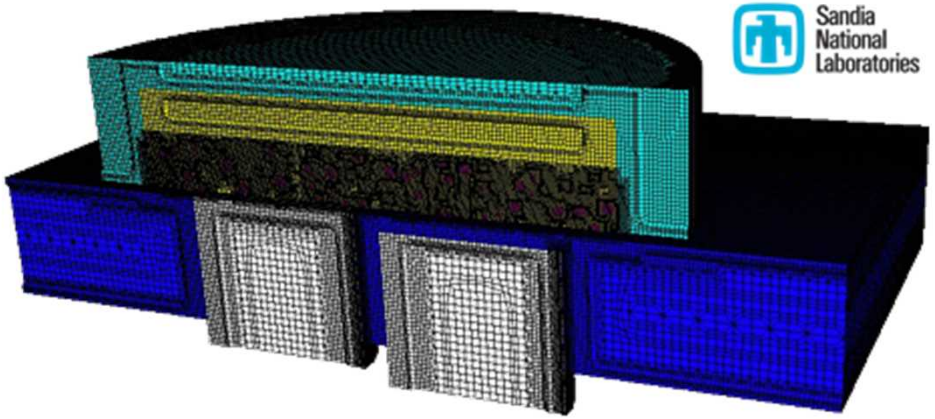


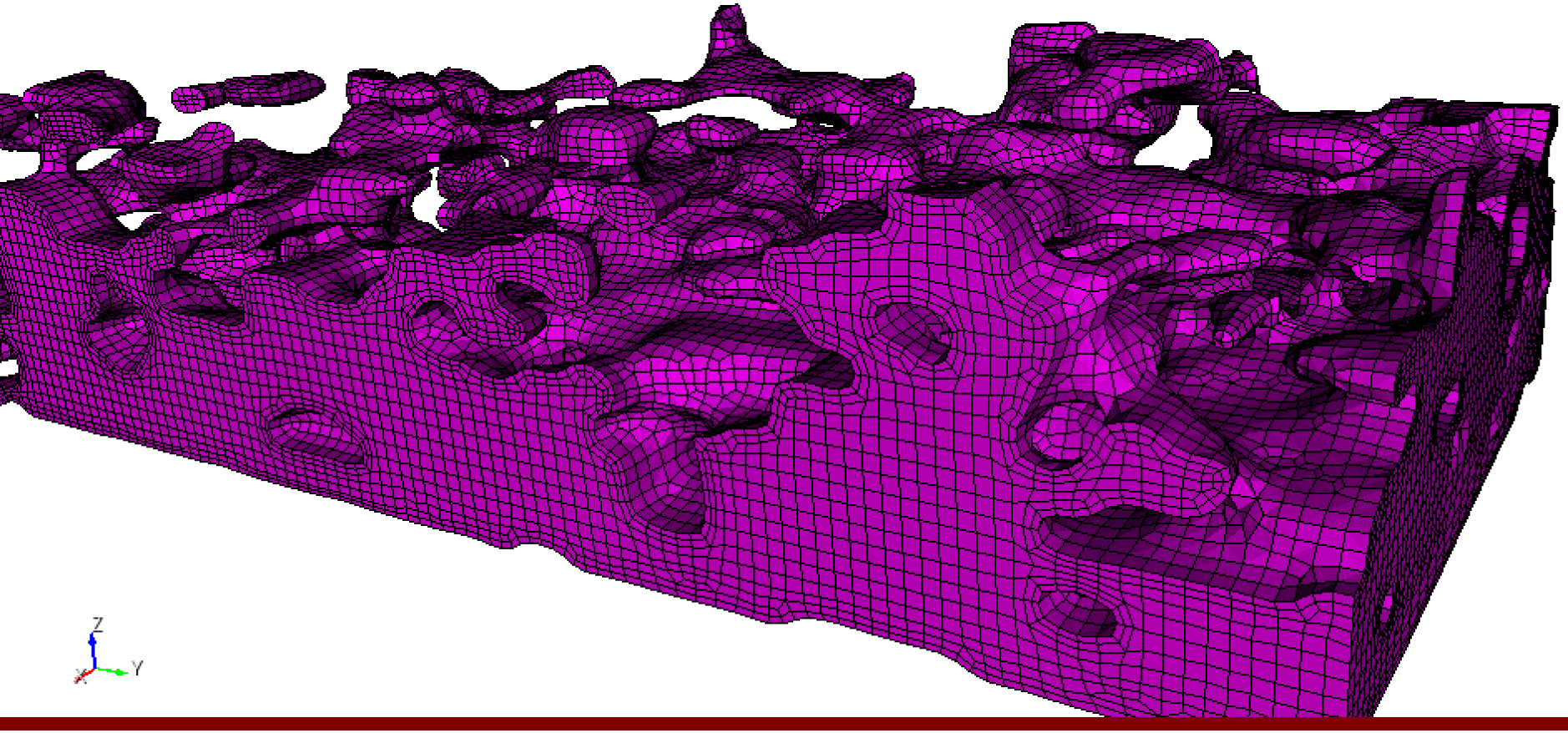


4 Refinement Levels
35,336,356 Hexes

Coarsening

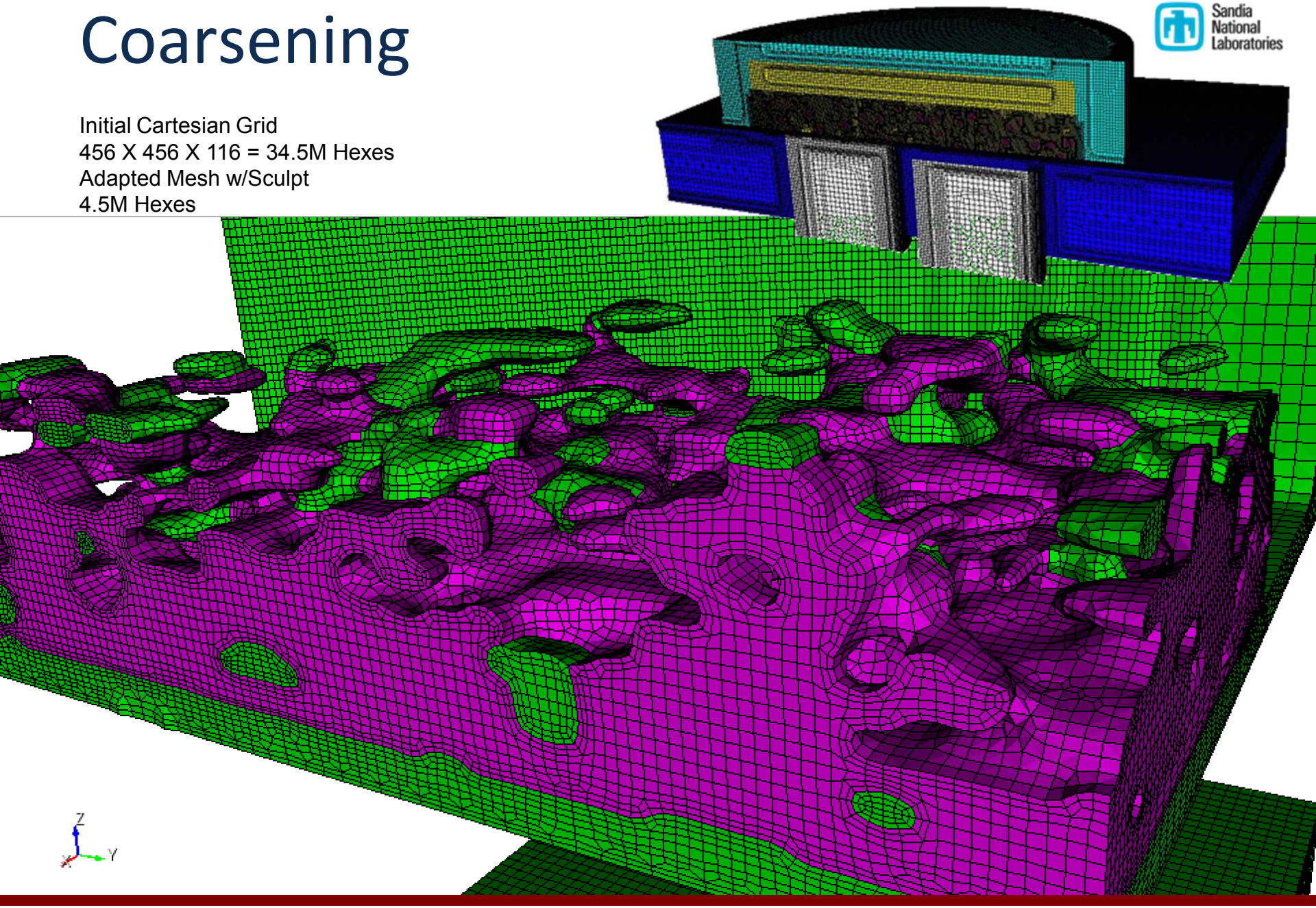
Initial Cartesian Grid
456 X 456 X 116 = 34.5M Hexes
Adapted Mesh w/Sculpt
4.5M Hexes





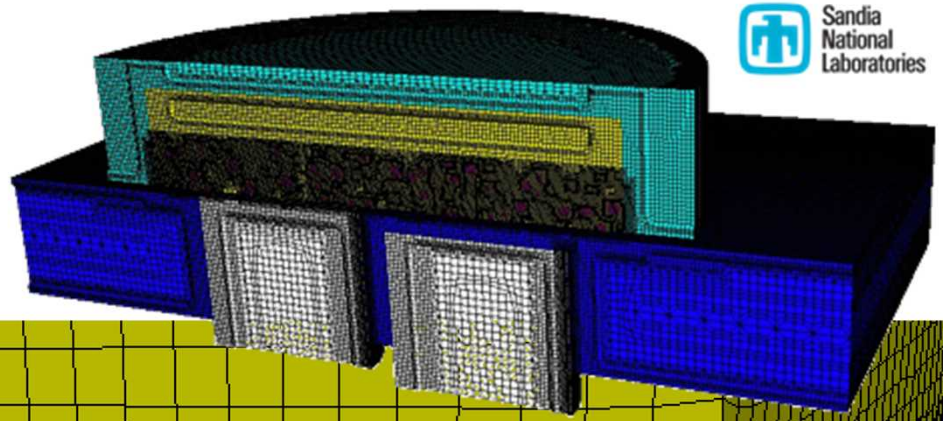
Coarsening

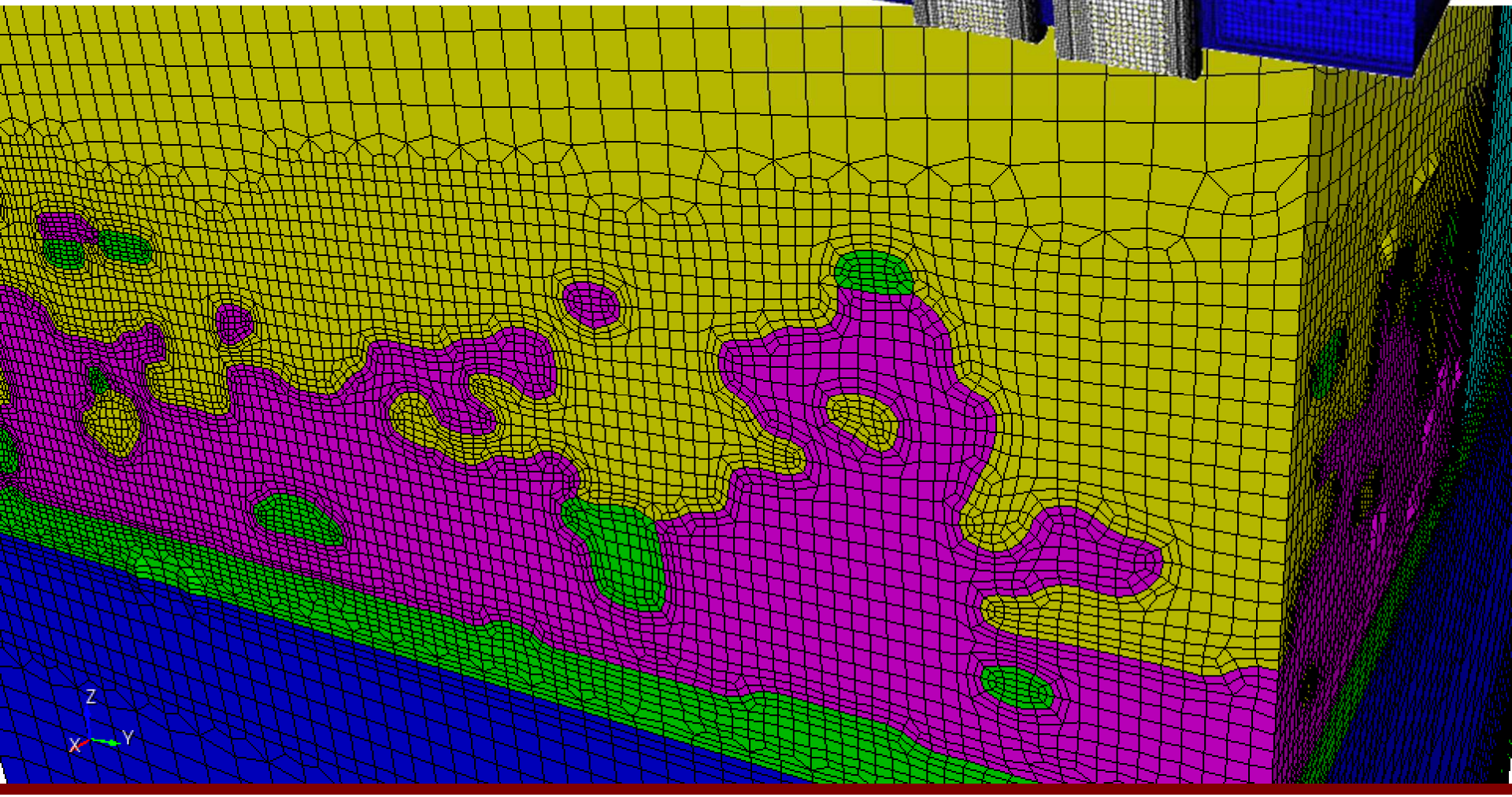
Initial Cartesian Grid
456 X 456 X 116 = 34.5M Hexes
Adapted Mesh w/Sculpt
4.5M Hexes



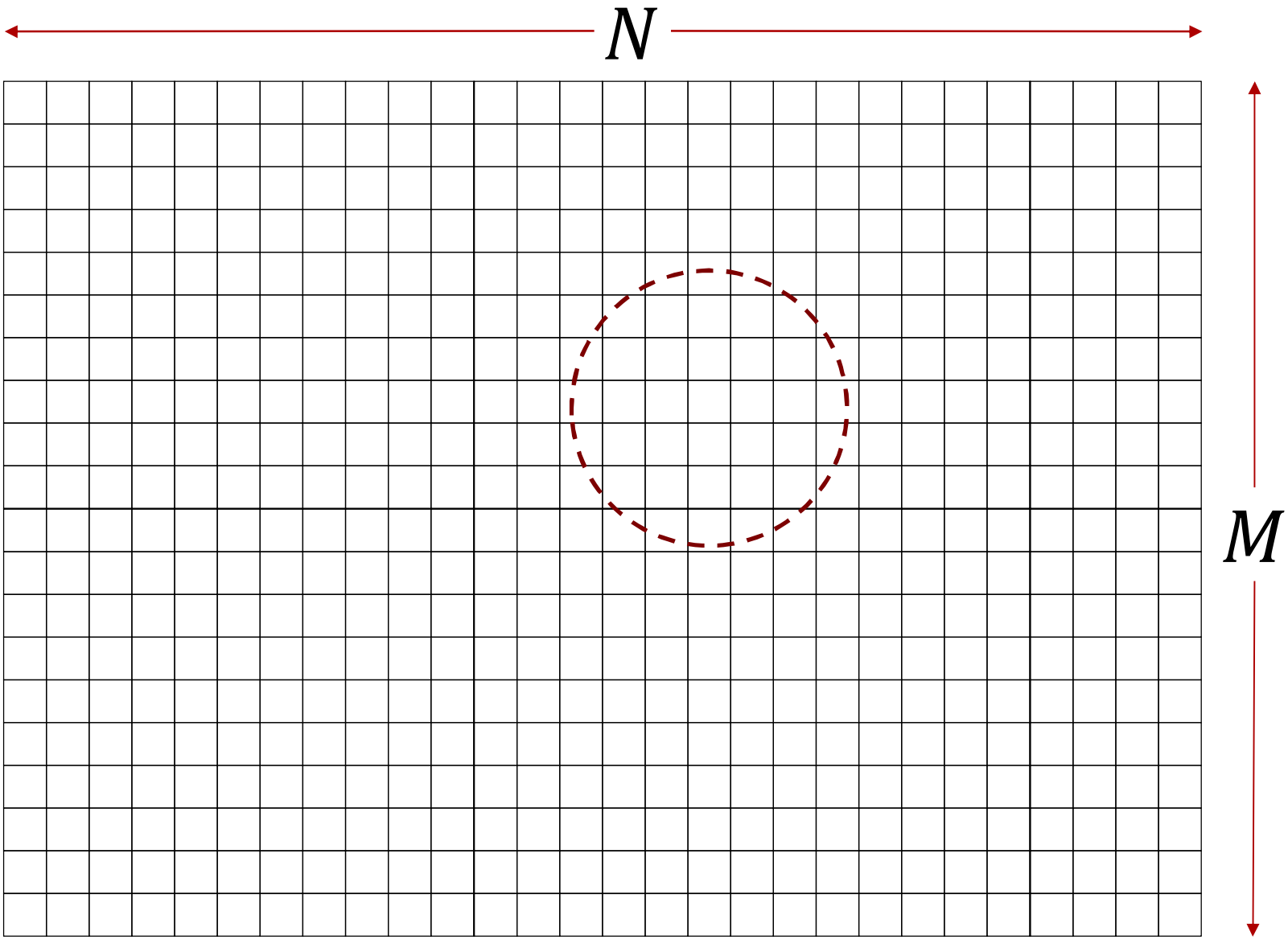
Coarsening

Initial Cartesian Grid
456 X 456 X 116 = 34.5M Hexes
Adapted Mesh w/Sculpt
4.5M Hexes

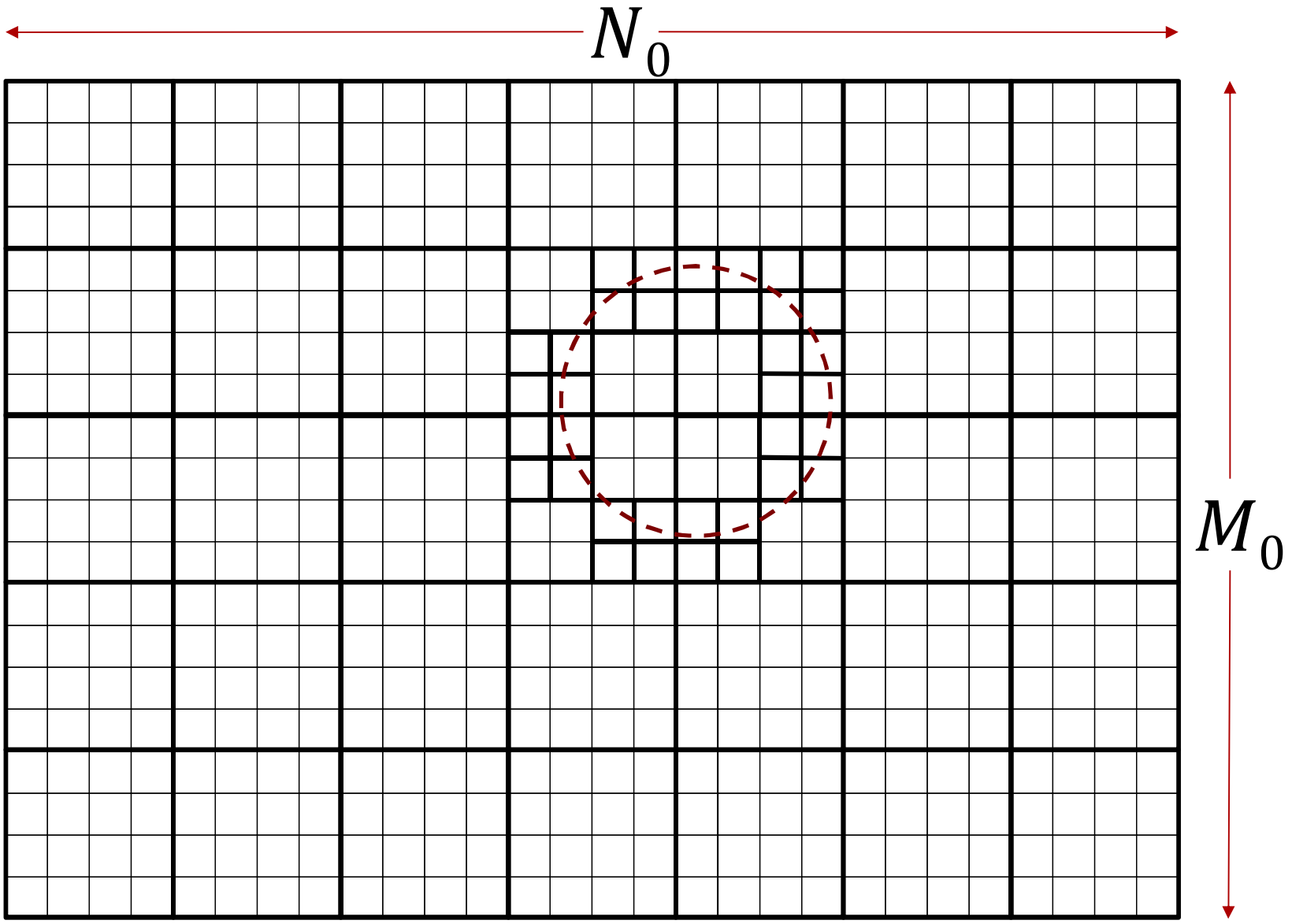




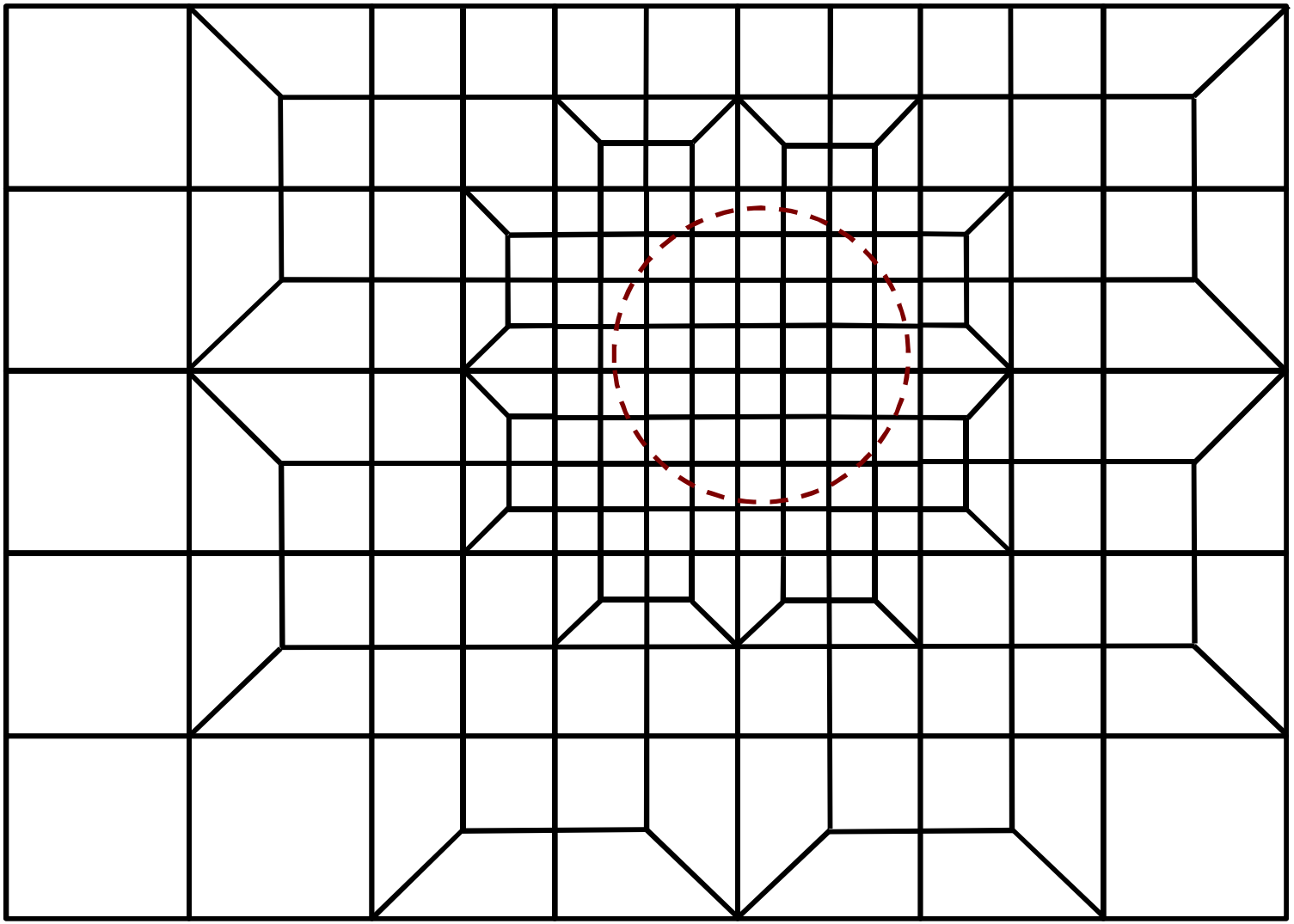
Coarsening



Coarsening

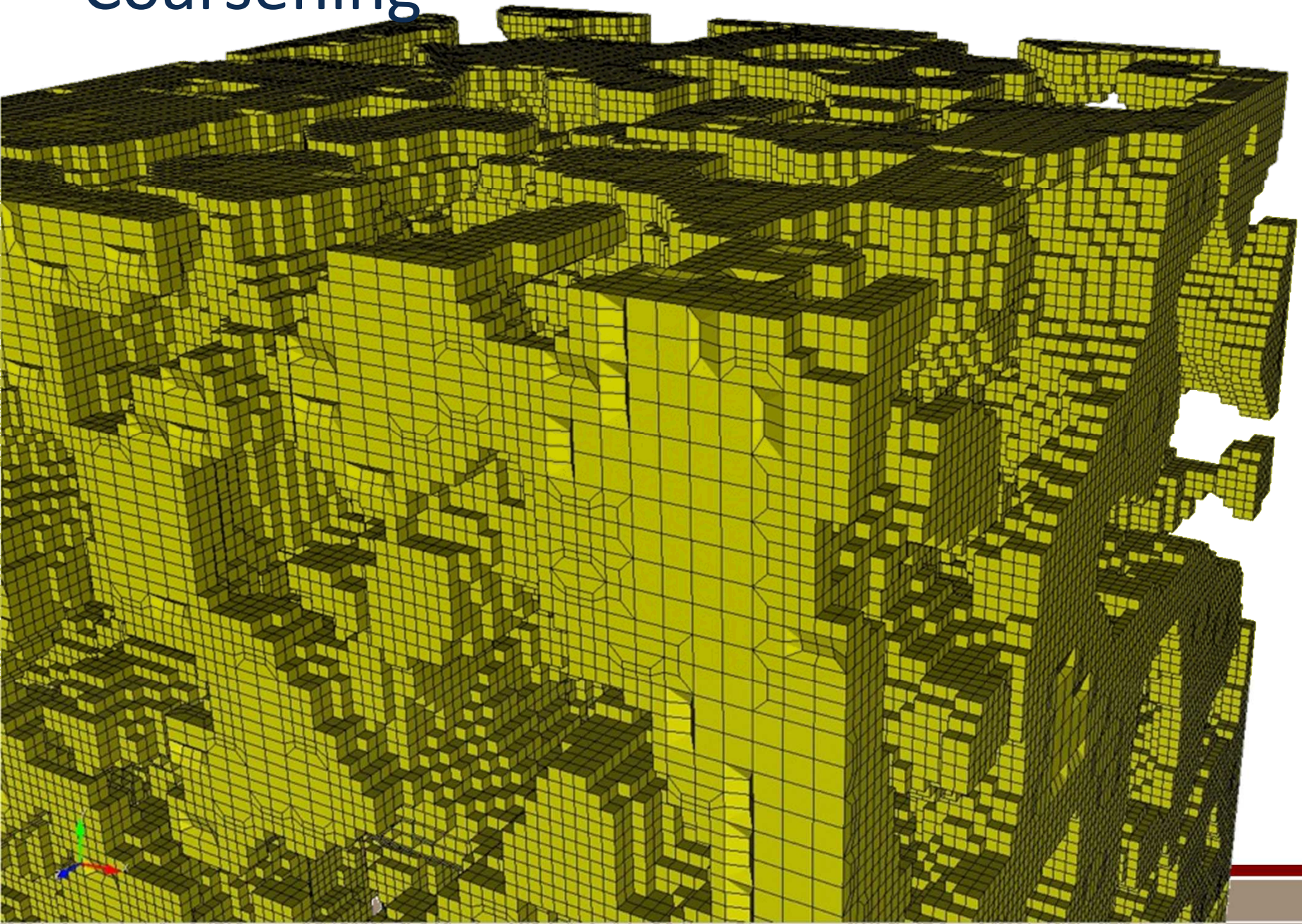


Coarsening

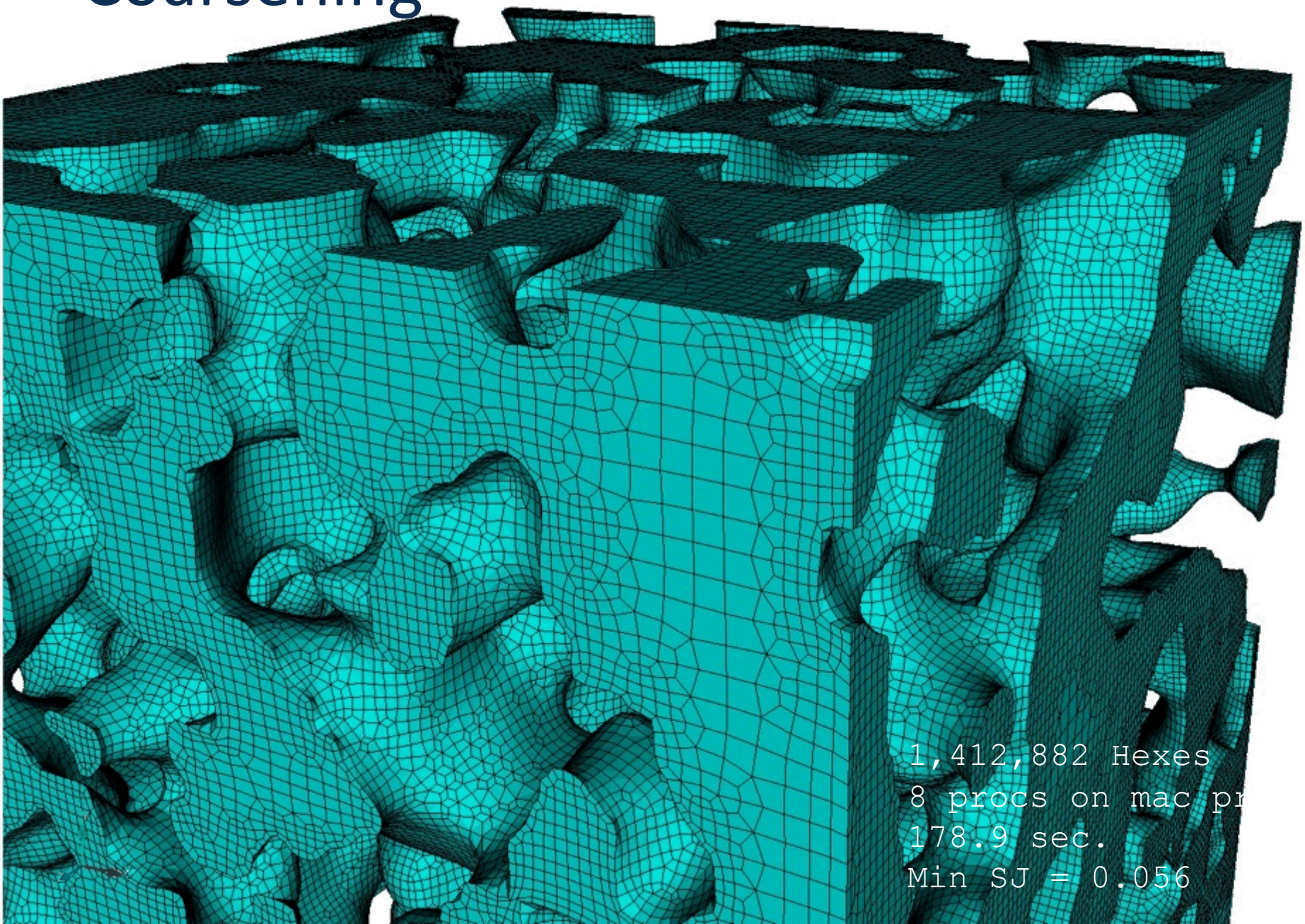


Coarsening

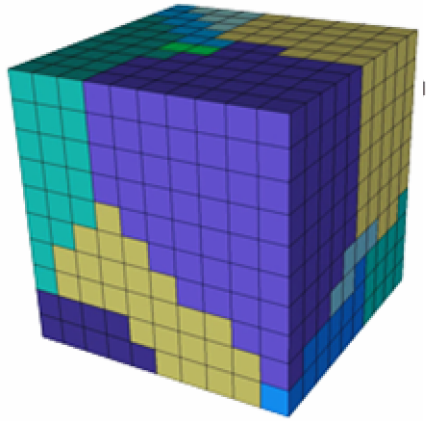
Sandia National Laboratories

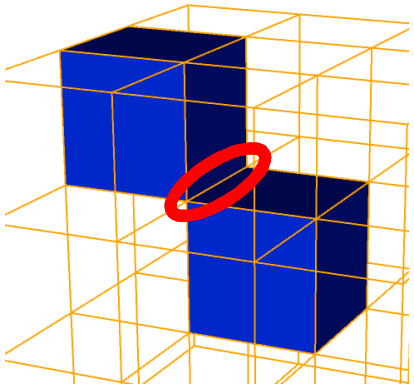


Coarsening

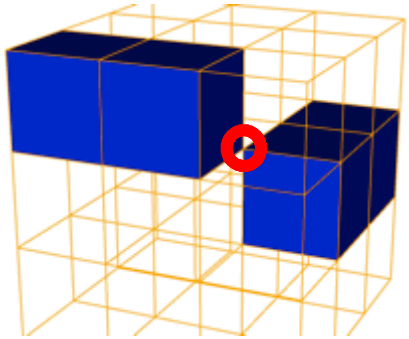


Non-manifold Resolution

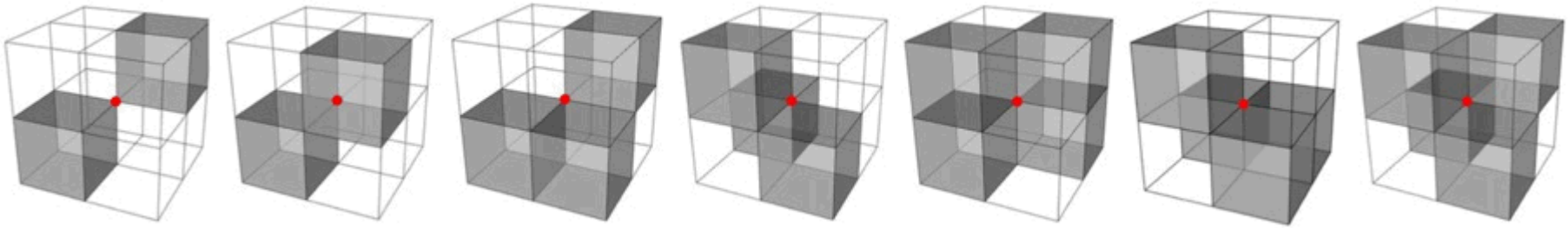




Non-manifold edge

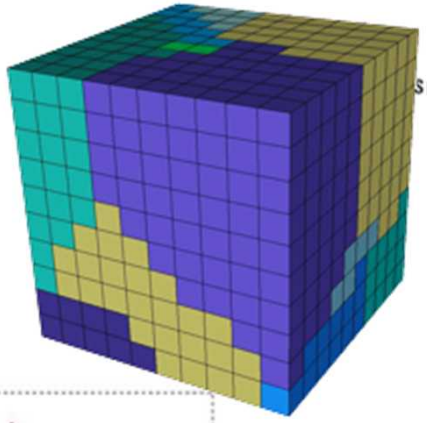


Non-manifold node



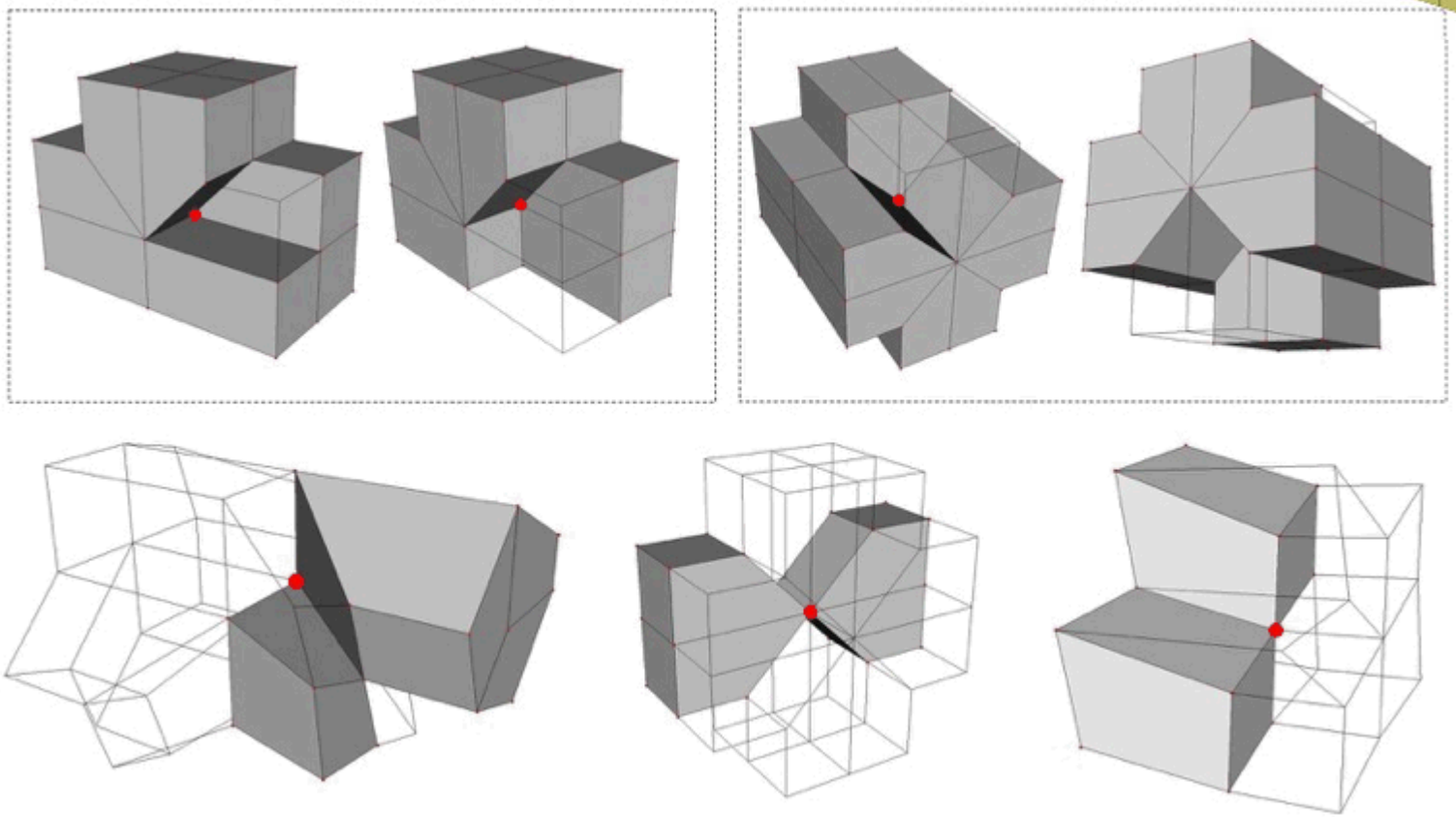
7 cases for Cartesian-Structured at a node

Non-manifold Resolution



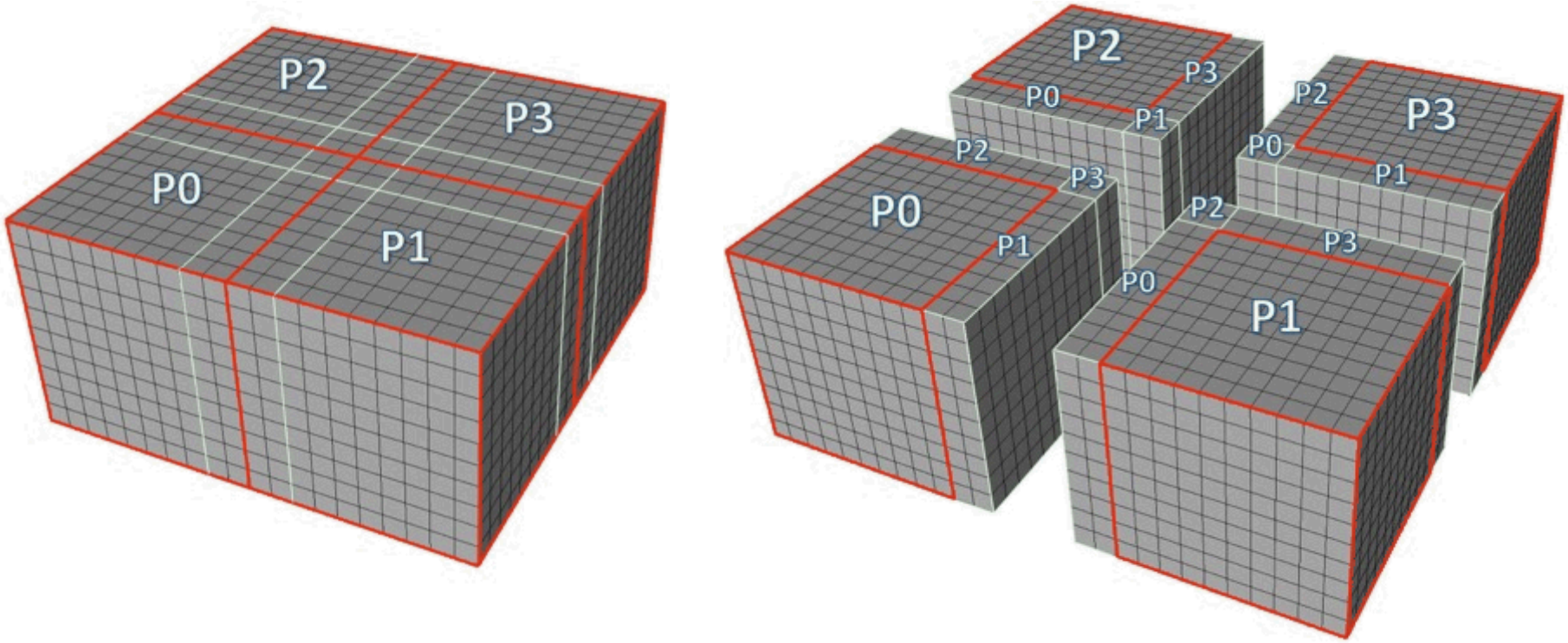
$$E = N_{nodes} - N_{edges} + N_{faces}$$

Euler Number $E \neq 2 \Rightarrow Non - manifold$



Many non-manifold cases for unstructured material at a node

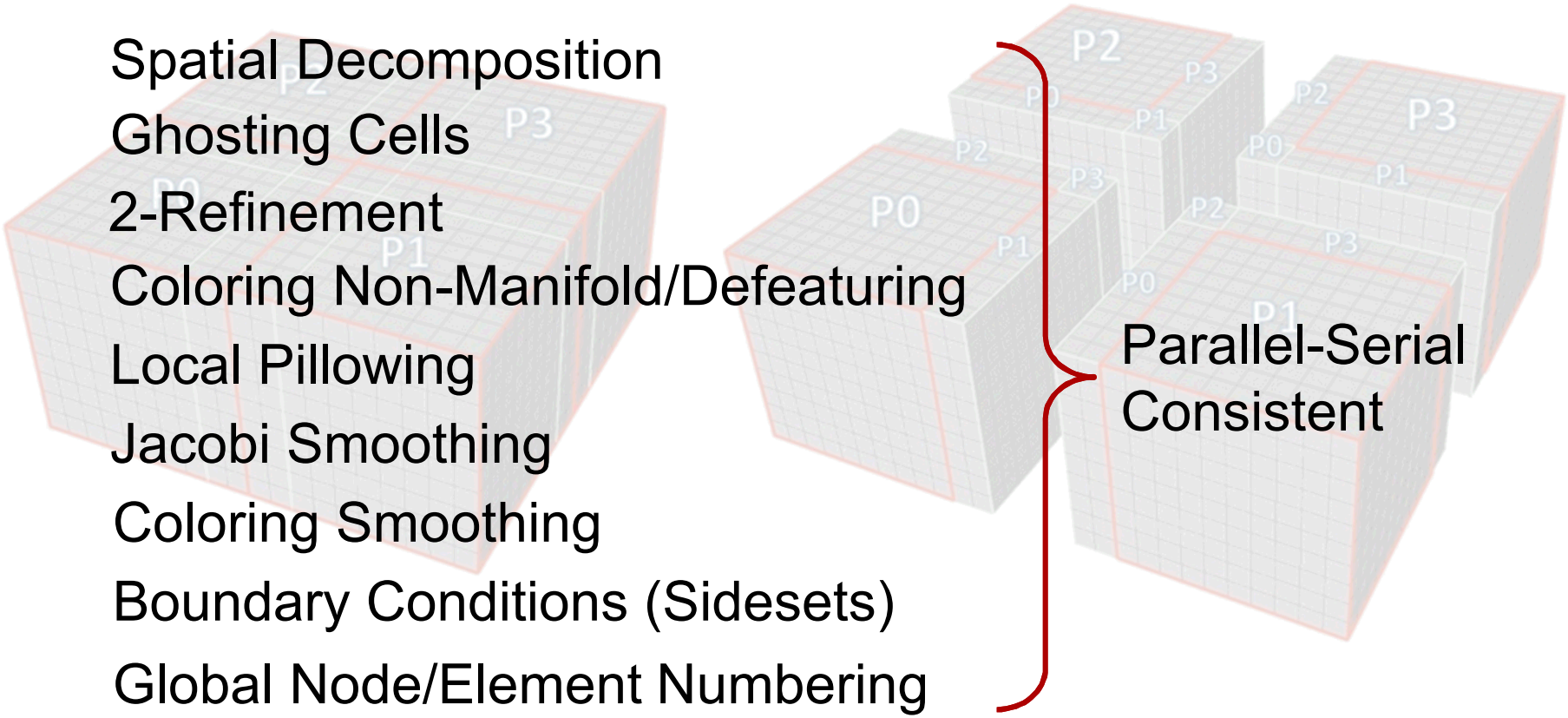
Parallel



Parallel

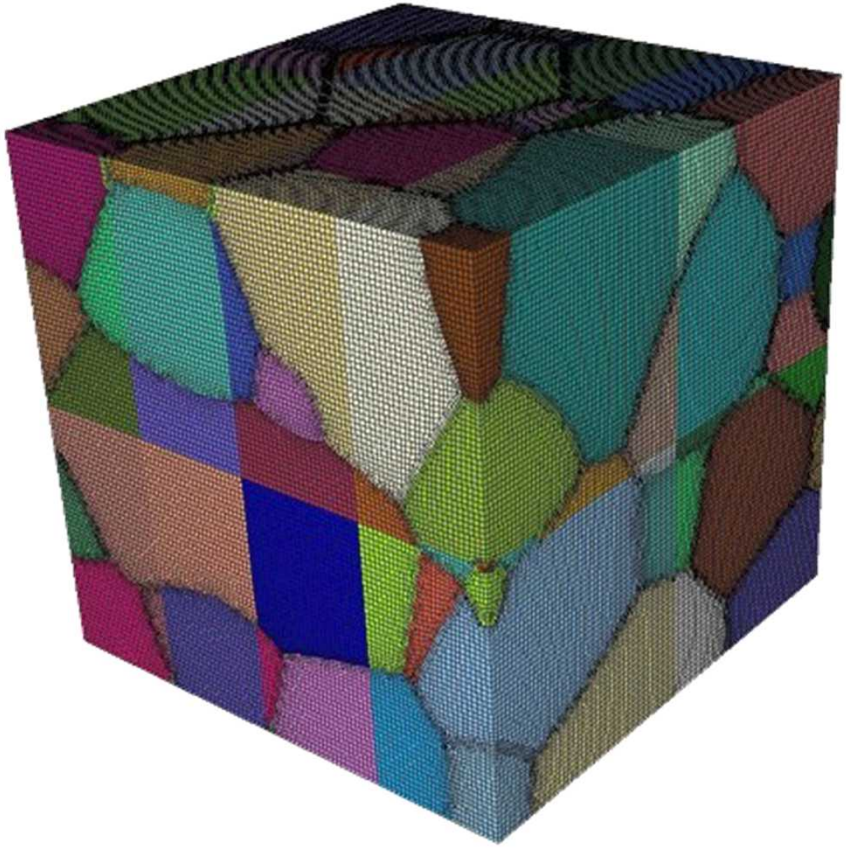
MPI Communcation

Spatial Decomposition
Ghosting Cells
2-Refinement
Coloring Non-Manifold/Defeaturing
Local Pillowing
Jacobi Smoothing
Coloring Smoothing
Boundary Conditions (Sidesets)
Global Node/Element Numbering

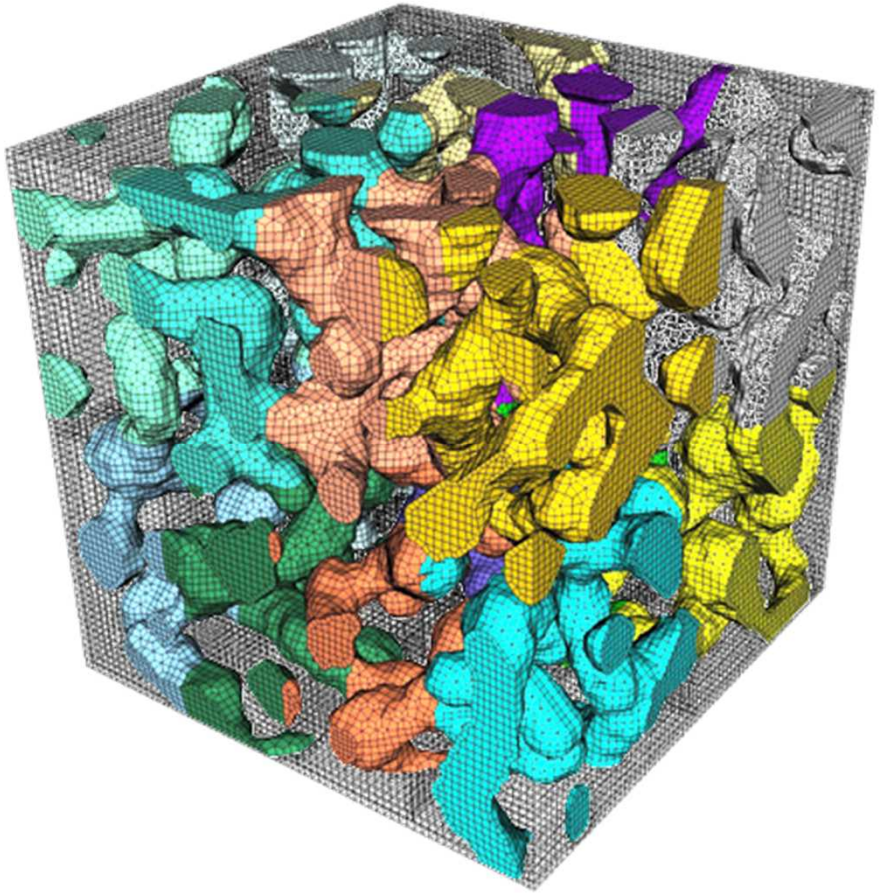


Parallel

Examples

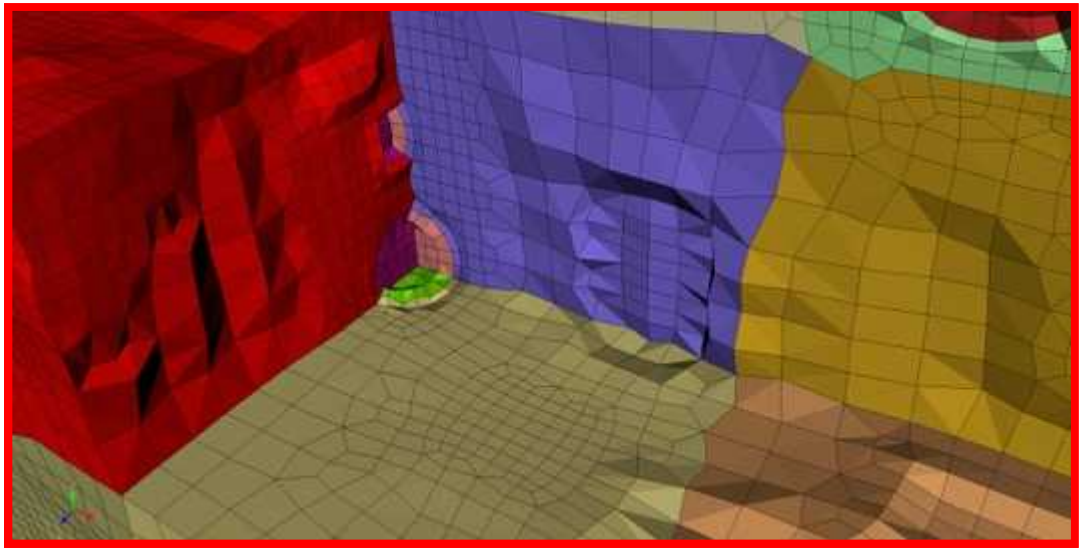


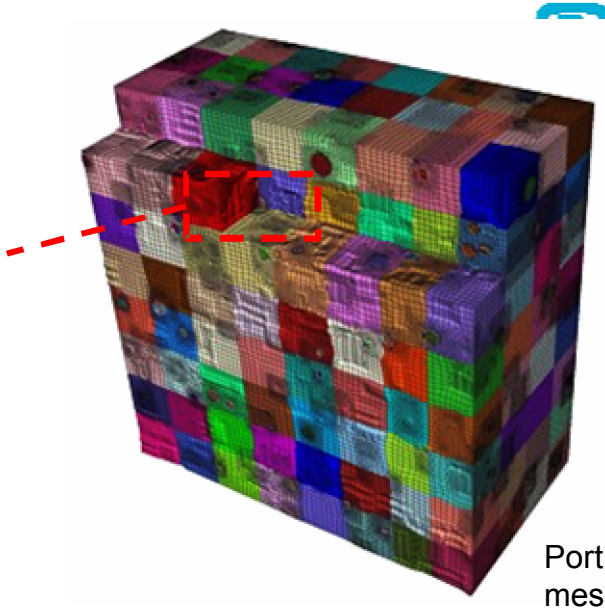
Microstructures with multiple unique volumes. 16 processors



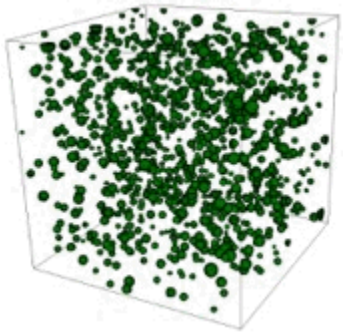
2 phase model. 16 processors

Parallel





Portion of mesh from 512 processors

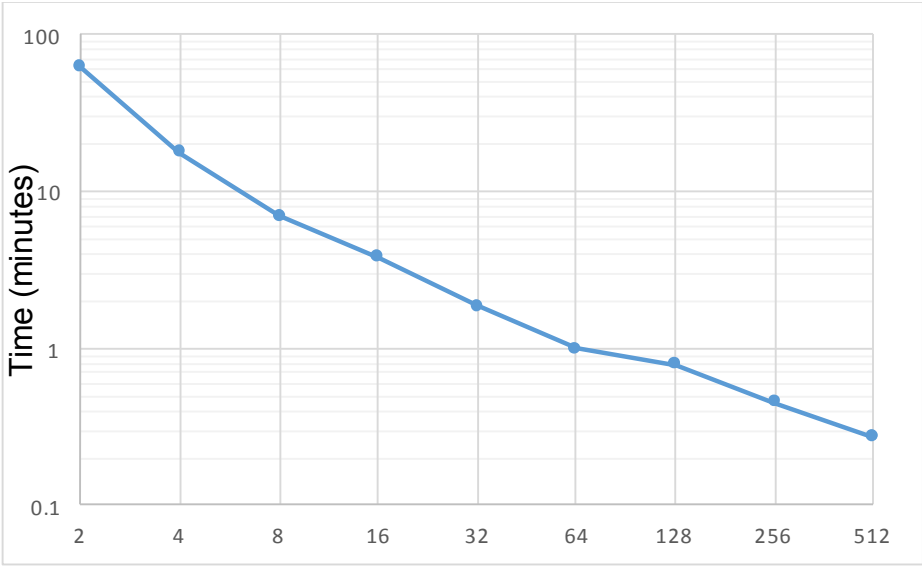


1300 Spheres
2 refinement Levels
Total Hexes 2,289,844

Tests performed on Sandia's Chama TLCC platform

Time to mesh RVE w/1300 spheres

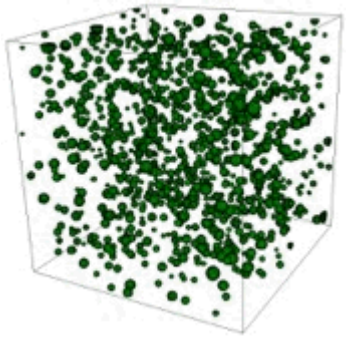
Num Procs	Time (minutes)
2	61.069
4	17.711
8	6.993
16	3.797
32	1.845
64	0.998
128	0.782
256	0.453
512	0.271

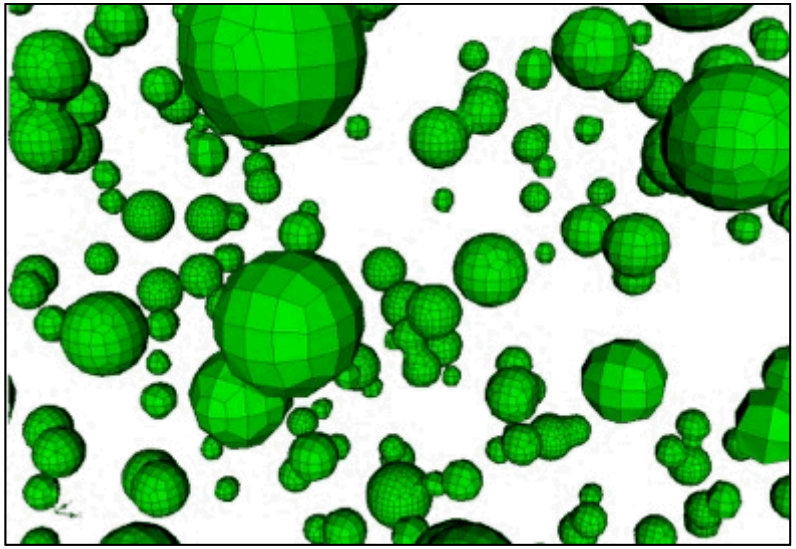


Example

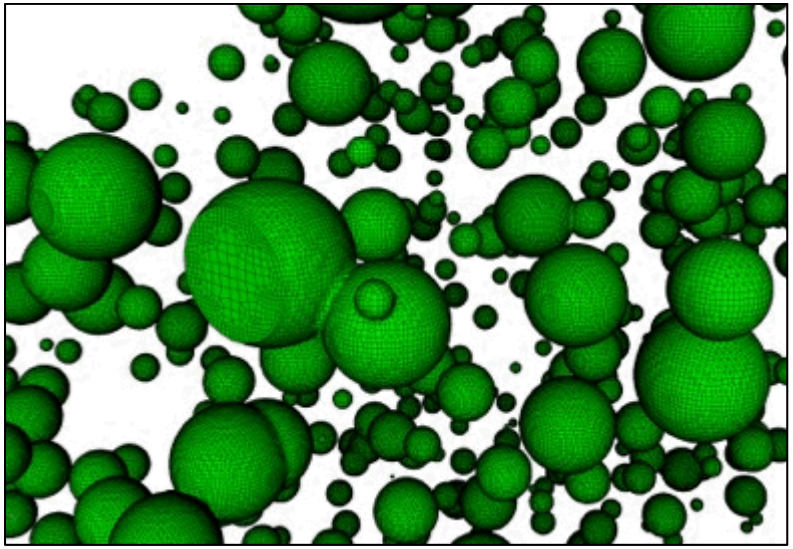
Refnement Levels	Num Hexes	Min S.J.	num hex < 0.2	Time (sec.)
1	3,614,934	0.1689	13	33.48
2	14,105,616	0.1334	21	192.4
3	50,278,564	0.1365	20	1015.4

128 Procs



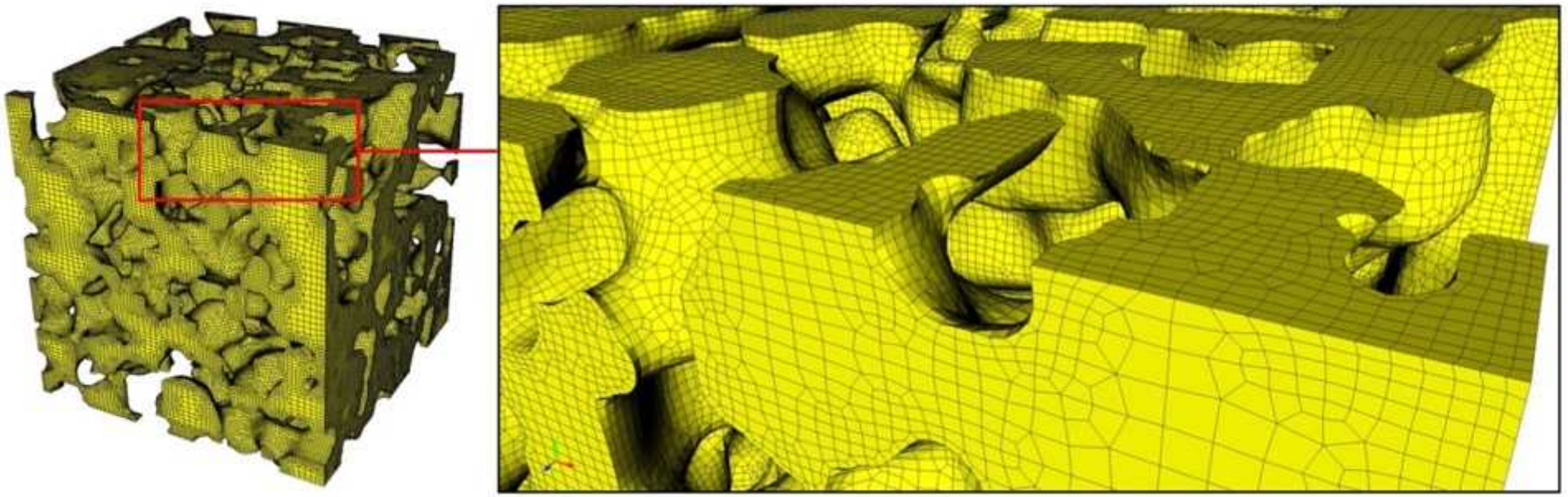


1 Refinement Level
3,614,934 Hexes

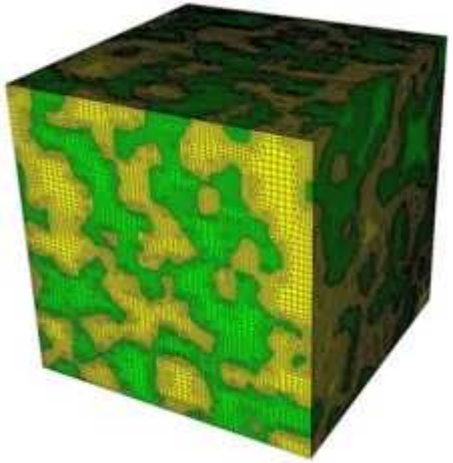


3 Refinement Levels
50,278,564 Hexes

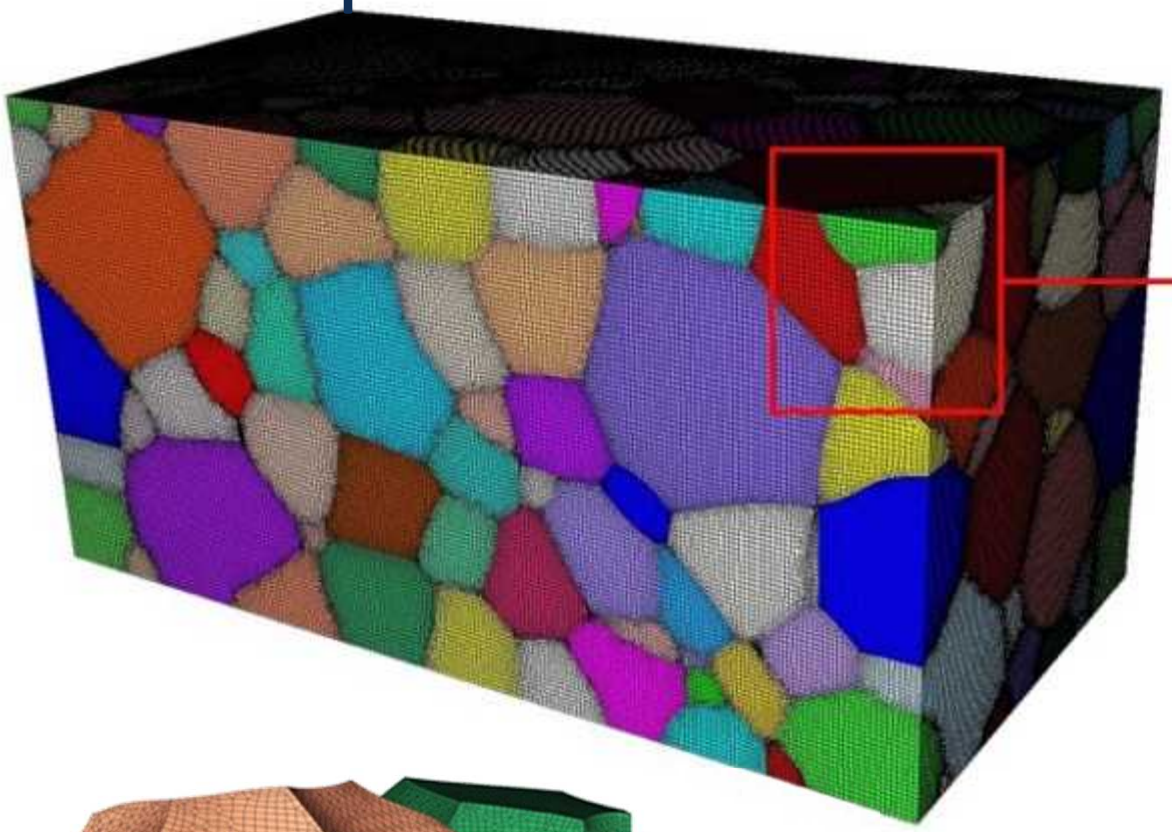
Example

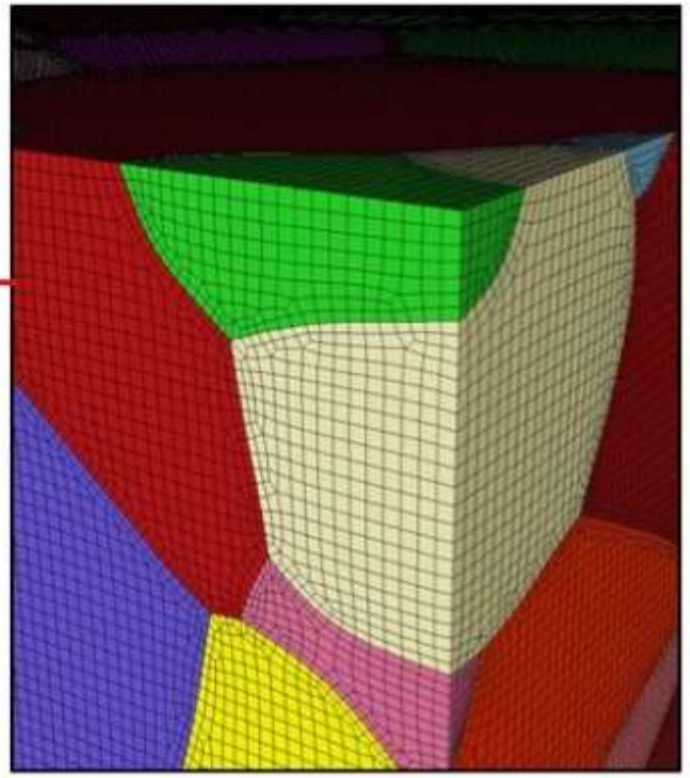


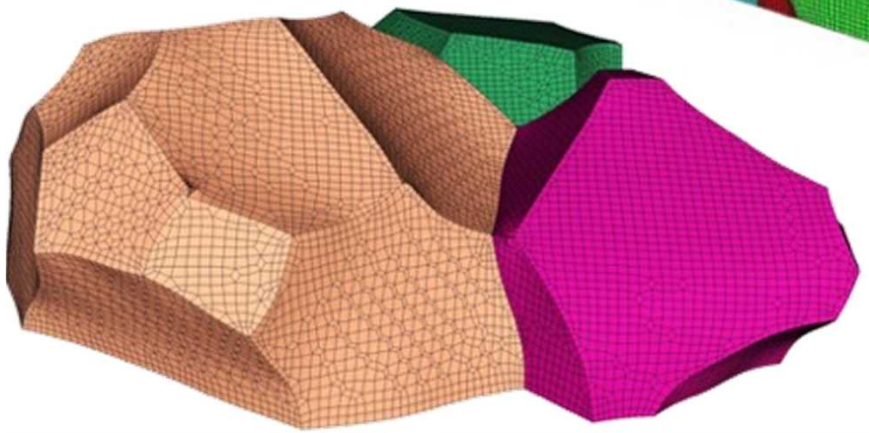
1 Refinement Level
Num Hexes = 1,412,340
Min. SJ. = 0.1211
Num Hexes < 0.2 = 11
Num Procs 8
Time = 181.2 sec.



Example







Num Materials = 143
Num Hexes = 3,655,878
Min. SJ. = 0.0749
Num Hexes < 0.2 = 73
Num Procs 12
Time = 201.2 sec.

Summary

- Toolkit for mesh generation for RVE models based on Sandia's **SCULPT** tool (Companion application to CUBIT)
- Input
  - Volume Fractions
  - Voxelated Cartesian
  - Analytic geometry
- Output
  - Exodus Mesh with Blocks and Sidesets
  - Faceted Geometry (Tet mesh in Cubit)
- Parallel – MPI
- Adaptive – Refinement and Coarsening
- Flitering/Defeaturing of Data
- Many applications and current materials R&D based on tool