LaGriT Mesh Generation and Model Set Up: Introduction

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EES-16 Computational Earth Science Earth & Environmental Sciences Division Los Alamos National Laboratory

http://meshing.lanl.gov

http://lagrit.lanl.gov



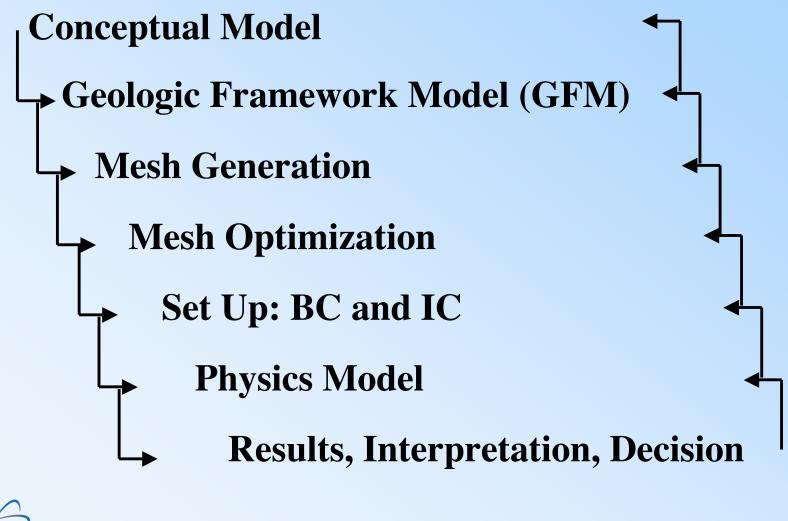
LaGriT Mesh Generation and Model Set Up

- LaGriT Los Alamos Grid Toolkit
- General meshing and setup, pre & post processing package
- Present examples from various geological applications
- http://lagrit.lanl.gov





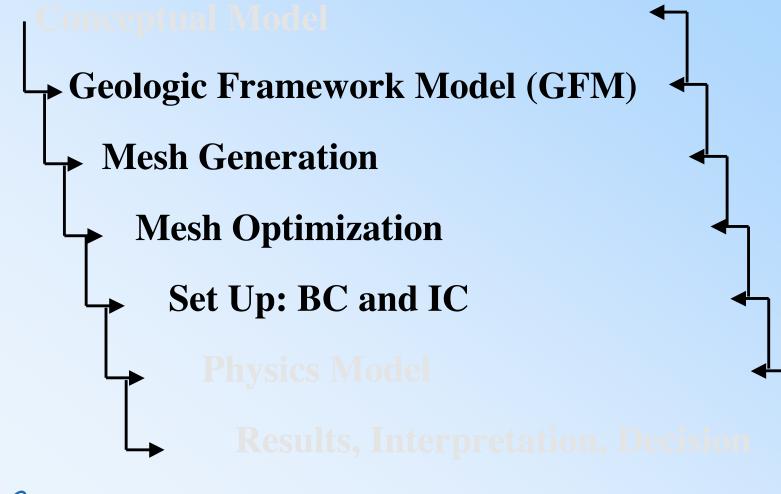
Geologic Modeling and Simulation Workflow







Geologic Modeling and Simulation Workflow







Geologic Framework Models (GFM) vs CAD

45km 150 faults 40 stratigraphic units Geologic model of Yucca Flat, Southern Nevada http://meshing.lanl.gov/proj

MNSX

Geologic Framework Models (GFM) vs CAD

v2.unsliced.faces

Geologic model of Yucca Flat

CAD Model





GFM Geologic

- 1. Geometry Poorly Known
- GASTON Stratamoust GAS of Strate of
- 4. Development driven by bit pate (high end), environmental (low end).
- 5. No symmetry
- 6. Often high aspect ratio 7. Non-manifold geometry dau

- **CAD Engineering**
 - 1. Geometry Know to High Precision

CAD Model (ACIS, Pro/E, Autocad) FE application well integrated Development of iven by automotive, aircraft, seniconductor, mechanical engineering, fluid dynamics Of en symmetry Often not high aspect ratio Manifold geometry: geometry defined by a set of air tight volumes





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• Los Alamos NATIONAL LABORATORY



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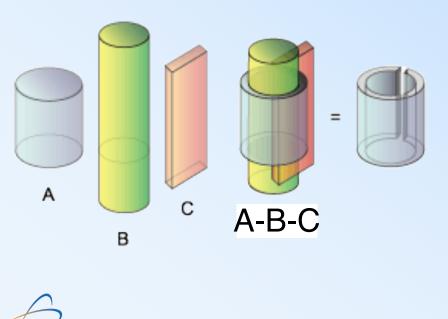
Forms of Geologic Framework Models (GFM) *Forms of Input to Meshing*

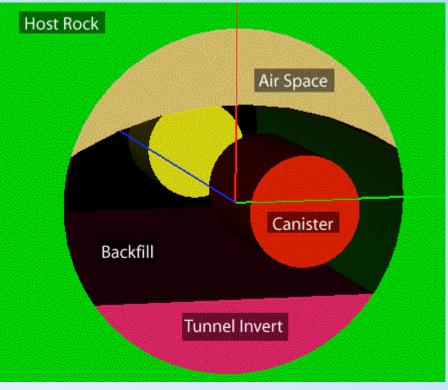
- Picture
- Map
- Cross Section
- Collection of surfaces that bound volumes
- Non-manifold Geometry
- Cellular model of 2D or 3D space (triangle, quadrilateral, hexahedral, tetrahedral, prism, pyramid, polygon, polyhedral)
- CAD
- Geologic modeling software





- Constructive Solid Geometry
- Collection of surfaces that bound volumes
- Can be used to define geometry, topology and attributes

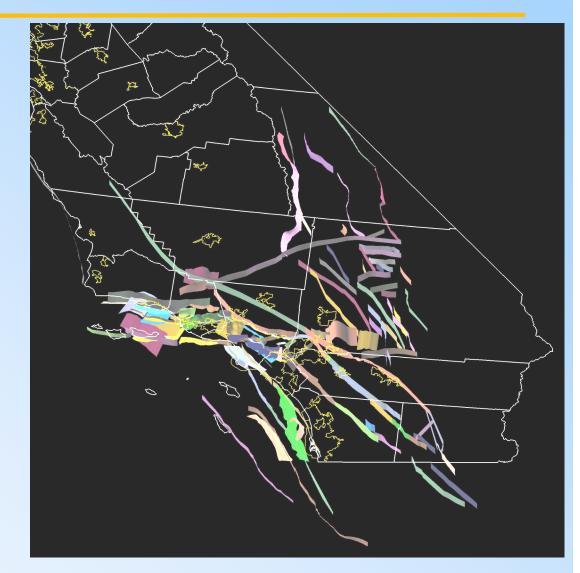








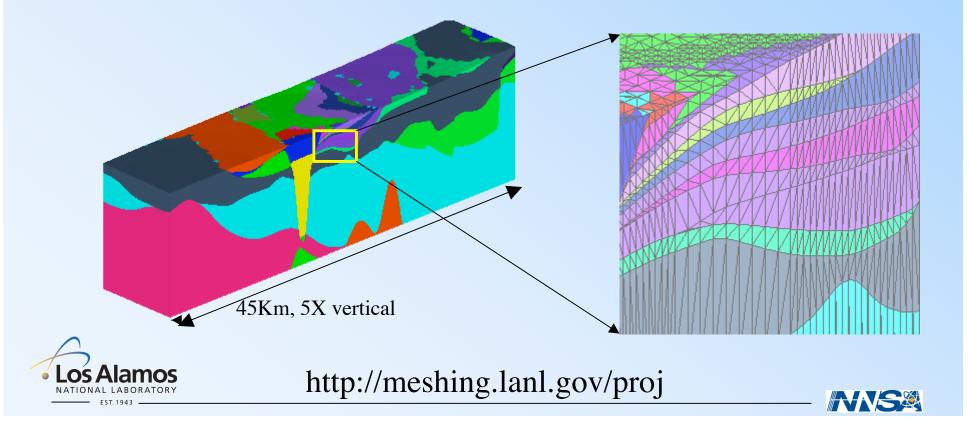
- Non-manifold Geometry
- Southern California Earthquake Center (SCEC) community fault model (CFM) of southern California
- Faults defined by triangulated surfaces
- Geometry of faults is well defined but topology is not defined







- Cellular model of 2D or 3D space (triangle, quadrilateral, hexahedral, tetrahedral, prism, pyramid, polygon, polyhedral)
- 3D geologic framework defined by tetrahedral elements



• Various Geologic Modeling Software Packages (EarthVision, gOcad/SKUA, Landmark, ...)

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http://meshing.lanl.gov/proj

EarthVision Model Southern Nevada



GFM Not in CAD Format

Option 1

- 1. Derive CAD solid model (ACIS, Pro/E, etc.) from geologic model (EarthVision, gOcad, Stratamodel, ...).
- 2. Use mesh generation tools that utilize CAD solid model input.

Option 2

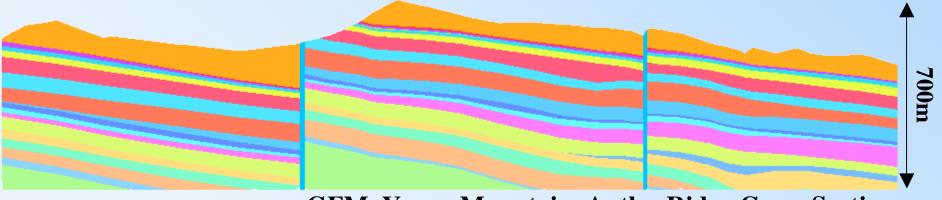
1. Use mesh generation tools that do not require CAD solid model input.





Mesh Generation Approach Depends on the Solver and Physics

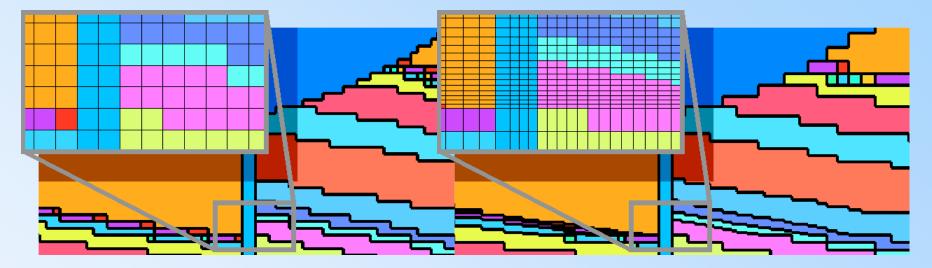
- Orthogonal Finite Difference, Logical Structured, Block Structured
- Quadtree, Octree
- 2.5 D Unstructured (*e.g.* stacked triangles)
- Unstructured (quad, tri, hex, tet, prism, pyramid, polyhedral)
- Mesh quality (aspect ratio, volume variation, ...)





GFM, Yucca Mountain, Antler Ridge Cross Section http://meshing.lanl.gov/proj

Mesh Generation: Orthogonal Finite Difference

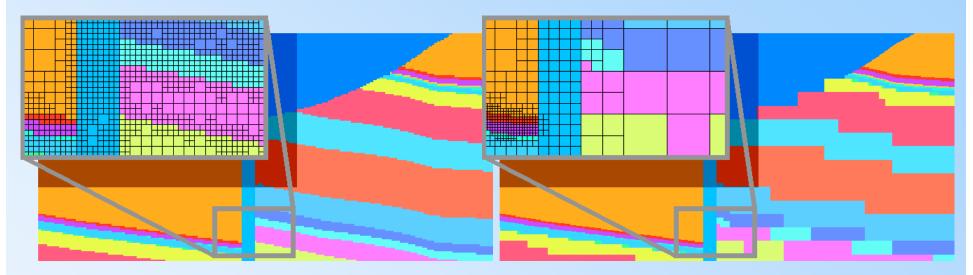


 Mesh node and element attributes are assigned from GFM but mesh resolution is not informed by GFM details





Mesh Generation: Adaptive Quadtree(2d)

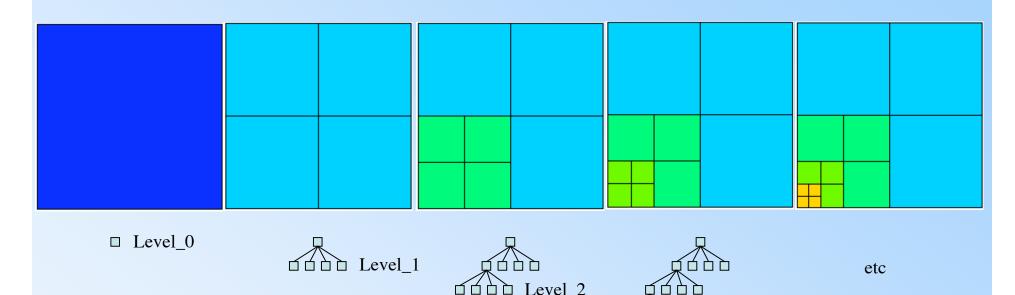


- Mesh node and element attributes are assigned from GFM
- Mesh refinement is informed by GFM geometry





What is a 2D QUADTREE, 3D OCTREE mesh?



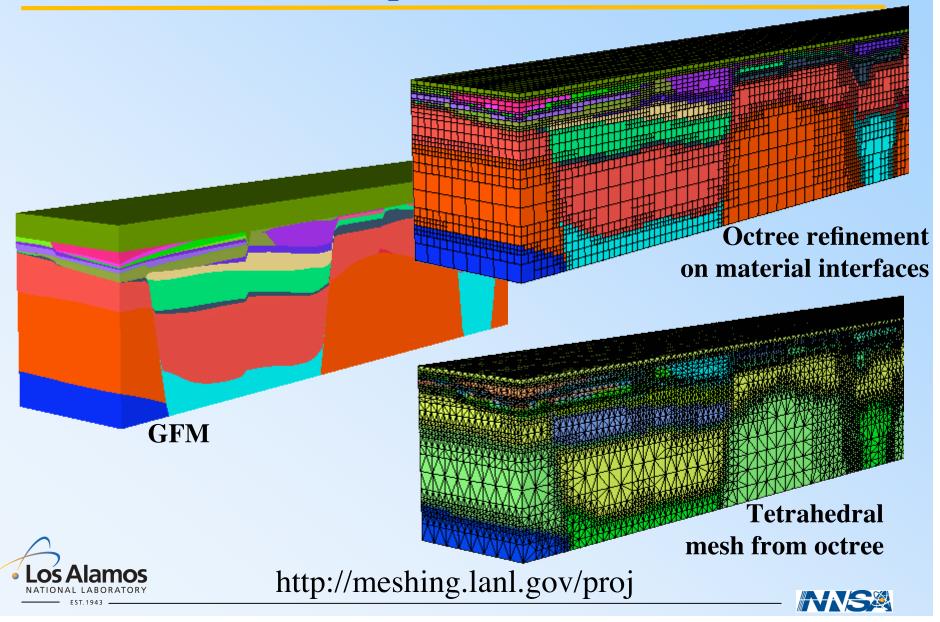
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- •Tree data structure, each branch has 4 leaves
- •Balance tree = level n has neighbors of level n-1, n, n+1
- •Octree is the 3D extension

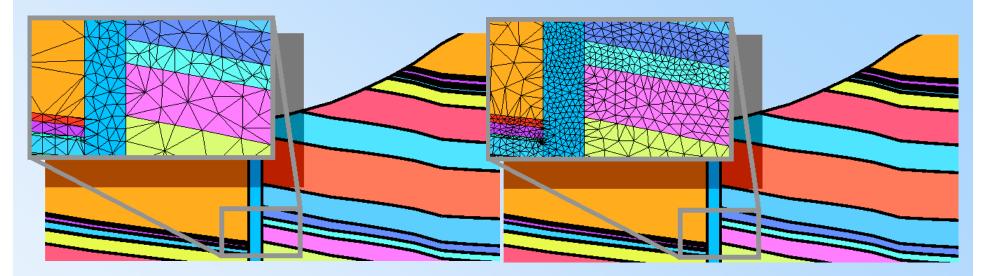




Mesh Generation: Adaptive Octree(3D)



Mesh Generation: Unstructured Triangle/Tetrahedral



- Mesh node and element attributes are assigned from GFM
- Mesh reproduces geometry and topology of GFM
- Mesh resolution is informed by GFM





Mesh Generation: Unstructured Tetrahedral (3D)

Southern California Fault Block Model (SCEC)

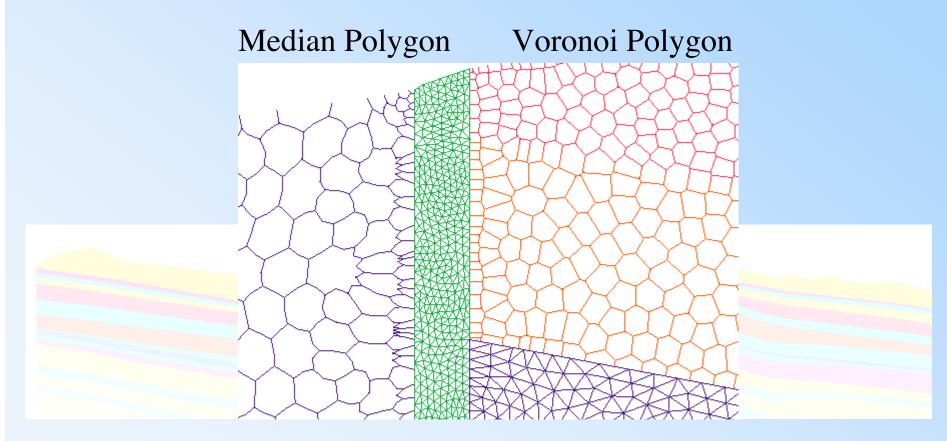
Alamos

- Mesh node and element attributes are assigned from GFM
- Mesh reproduces geometry and topology of GFM
- Mesh resolution is informed by GFM



Mesh Generation Depends on the Solver and Physics

• Unstructured polyhedra (control volume methods)







Model Setup: Attributes, Boundary and Initial Conditions

GFM to Mesh Interpolation

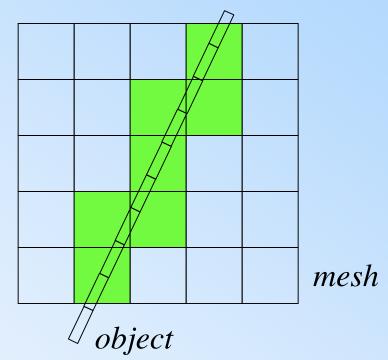
- Set material properties to nodes and/or elements (*e.g.* density, permeability)
- Set boundary conditions from GFM or another model (*e.g.* boundary flux)
- Upscale
 - Interpolate fine mesh properties onto a coarse mesh with various options for upscale function.
- Mesh-Object Intersections
 - Point (injection), line (well bore), surface (fault), volume (tunnel)





Mesh-Object Intersection

Compute intersection of *object* with *mesh*



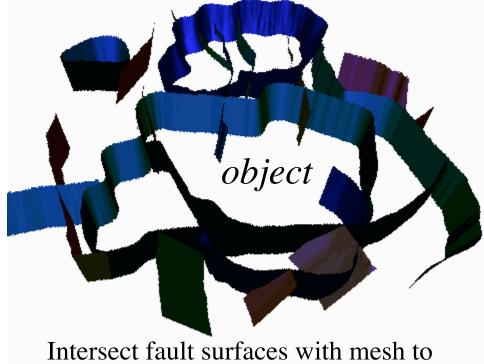
Mesh-Object Intersections: Point (injection), line (well bore), surface (fault, stratigraphic boundary), volume (tunnel, ore body, plume)





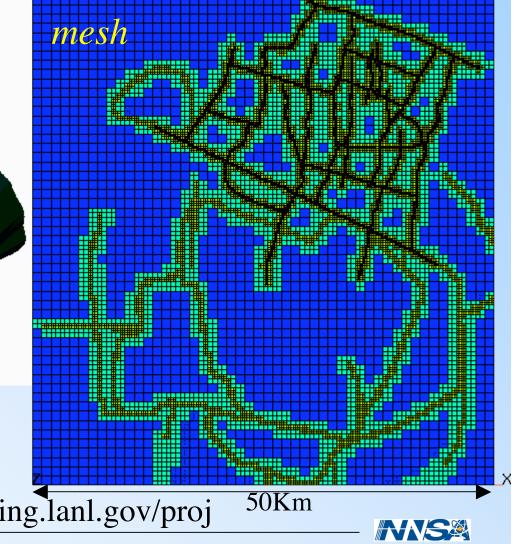
GFM Object - Computational Mesh Intersect/Refine

Compute intersection of *object* with *mesh*, refine mesh

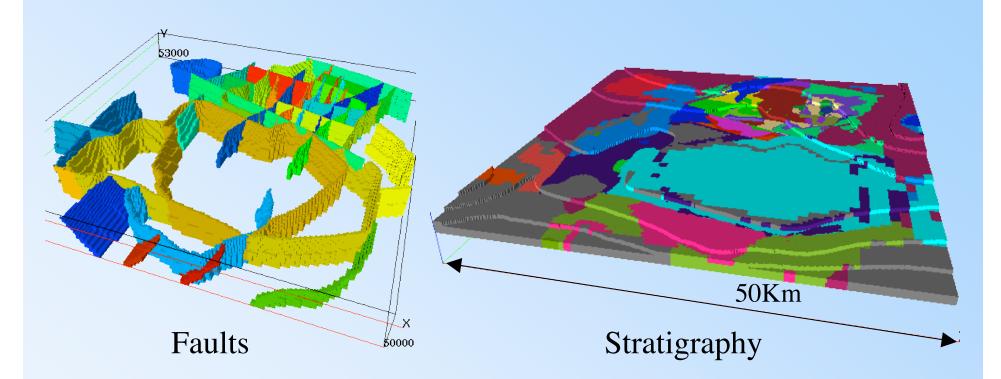


select elements to be refined with quadtree type mesh refinement.





3D Octree Refined Mesh



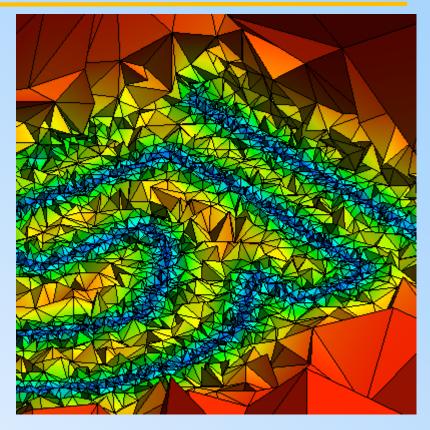




Mesh Optimization: Adaptive mesh refinement



Mesh resolution depends on a field $f(\underline{x})$, such as distance from model feature. Requires calculation of distance field $d=dist(\mathbf{q},\mathbf{p}_i)$, where d denotes the minimum distance from a point q to the nearest point on object \mathbf{p}_i .

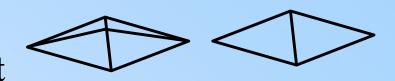


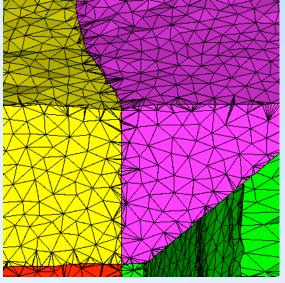




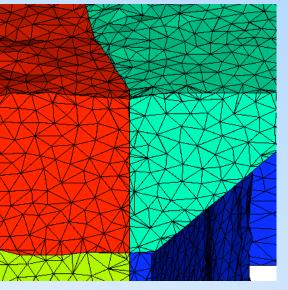
Mesh Optimization

• Refine, Derefine, Smooth – edge length, volume, aspect





Original Elements



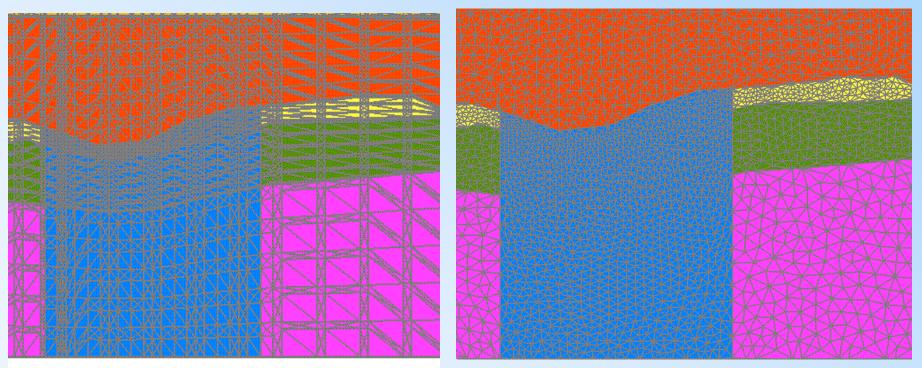
Remove small area/volume and high aspect ratio elements while maintaining geometry.





Mesh Smoothing

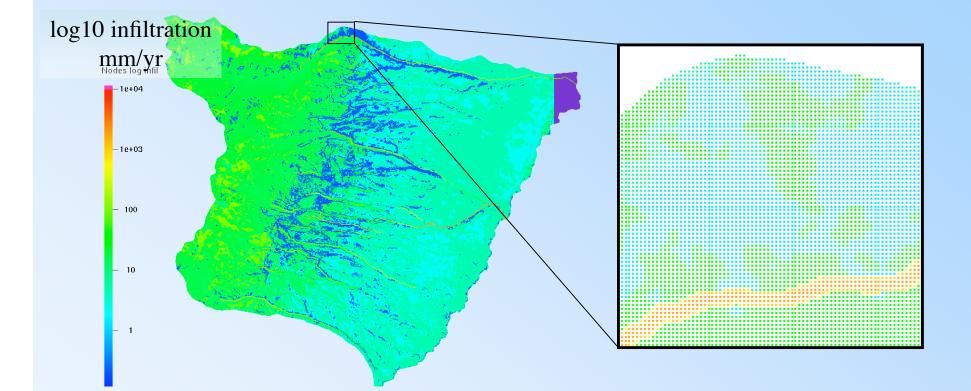
- Smooth 2D and 3D
 - elliptic, laplace, aspect, ...







Mesh to Mesh Interpolation

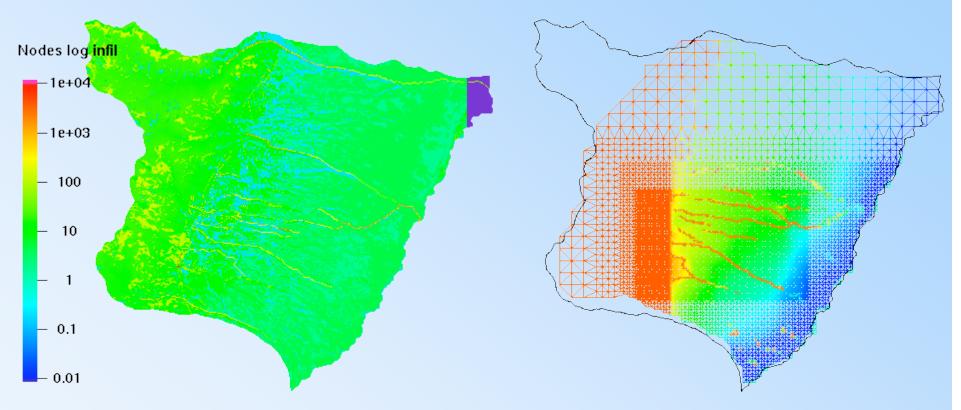


• Infiltration (mm/yr) map on regular mesh.





Mesh to Mesh Interpolation



• Infiltration boundary condition (right) based on mass conserving interpolation from a high resolution mesh to a lower resolution computational mesh for flow model.





Moving Finite Element Simulation of Thermally Driven Grain Growth

Physics code interacts with mesh seneration software to manage evolution of tetrahedral elements by maintaining mesh quality and topological changes associated with elimination of grains.

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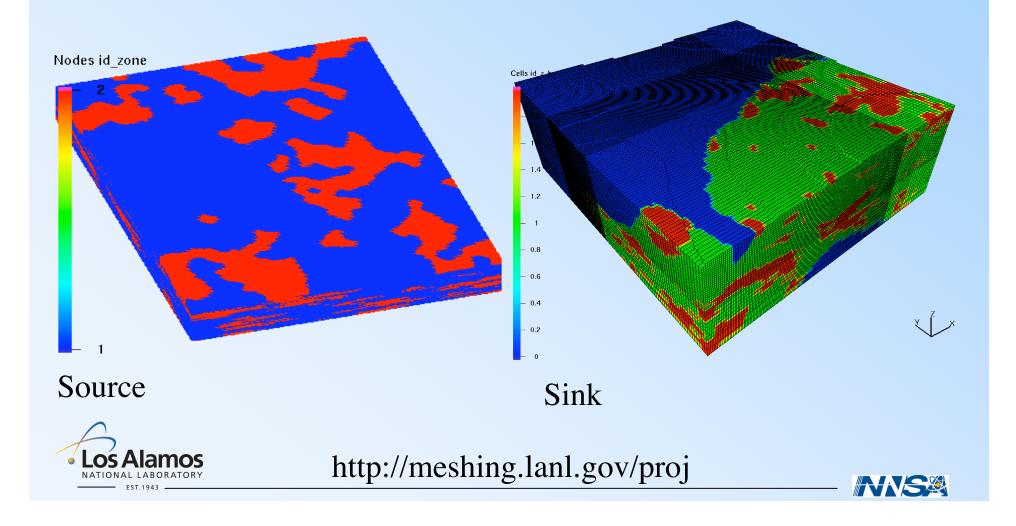


http://meshing.lanl.gov/proj

Calculation by Andrew Kuprat



•Interpolate scalar quantity (head, concentration, geostatistical property distribution) from one mesh to another



LaGriT

- •No GUI
- •3 Ways to Run LaGriT
 - •Command line: read / gmv / points.gmv / mol connect
 - dump / gmv / tets.gmv / mol
 - •Command File: lagrit < input.lgi
 - •Call from C or Fortran Code:
 - string = `read / gmv / points.gmv / mol'
 call dotask(string,error_flag)





LaGriT

Mesh Object: A data structure that contains geometry, topology and attributes

- Node geometry, x, y, z
- Mesh topology, connectivity of line, tri, quad, prism, pyramid, tet, hex elements
- Attributes (pressure, temperature, color): integer or real quantities on nodes or elements
- Point sets
- Element sets
- Neighbor Information
- Other book keeping...

LaGriT allows you to have many mesh objects simultaneously





LaGriT

Command Line Syntax (<u>http://lagrit.lanl.gov/docs/conventions.html</u>)

•Lines are a maximum of 80 characters long

•Continuation lines are signaled by an "&" as the last character of a line to be continued. A command can be up to 1024 characters long.

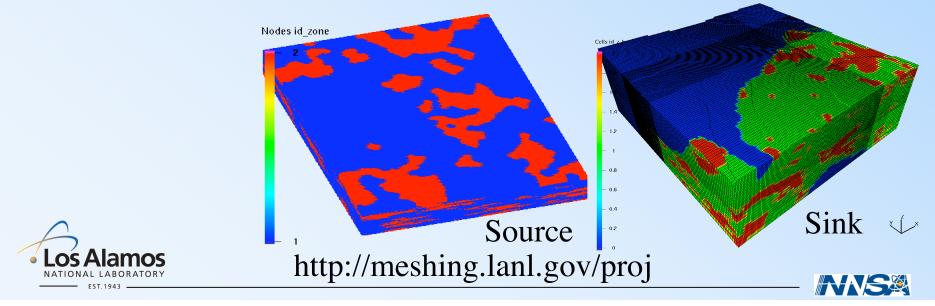
- •Delimiters are comma, slash, equal sign, or blank. (',' '/' '=" ').
- •Commands should be typed in lower case, however names are case sensitive.
- •To separate commands on the same line use a semicolon (;).
- •Three coordinate systems are used, xyz, rtz, rtp.





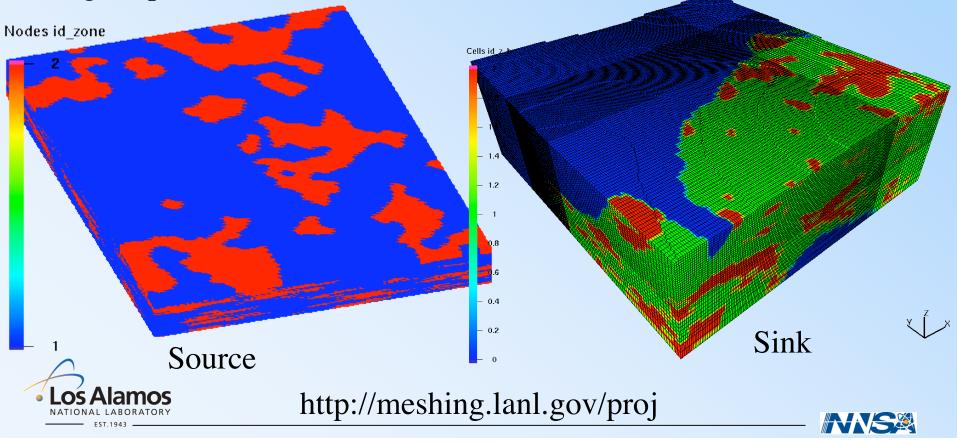
Interpolate scalar quantity (head, concentration, geostatistical property distribution) from one mesh to another cmo/readatt/source_mesh / xic yic zic id_zone id_elem /1,0,0 / file1 read / gmv / file2 / sink_mesh pset /pinterp1/ attribute / imt / 1 0 0 / 10 / eq interpolate / voronoi / sink_mesh / id_z_a / pset get pinterp1 / source_mesh / id_zone pset / pa_1 / attribute / id_z_a / 1 0 0 / 1 / eq pset / pa_2 / attribute / id z a / 1 0 0 / 2 / eq

- pset / pa 1 / zonn / outfile1.zonn / ascii
- pset / pa_2 / zonn / outfile2.zonn / ascii

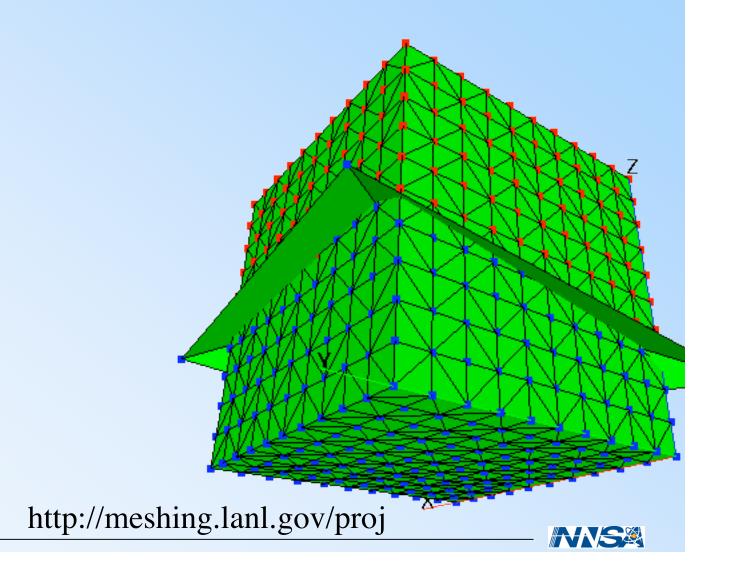


•Interpolate scalar quantity (head, concentration, geostatistical property distribution) from one mesh to another

•Accelerated implementation using a kd-tree search resulting in NlogM speed

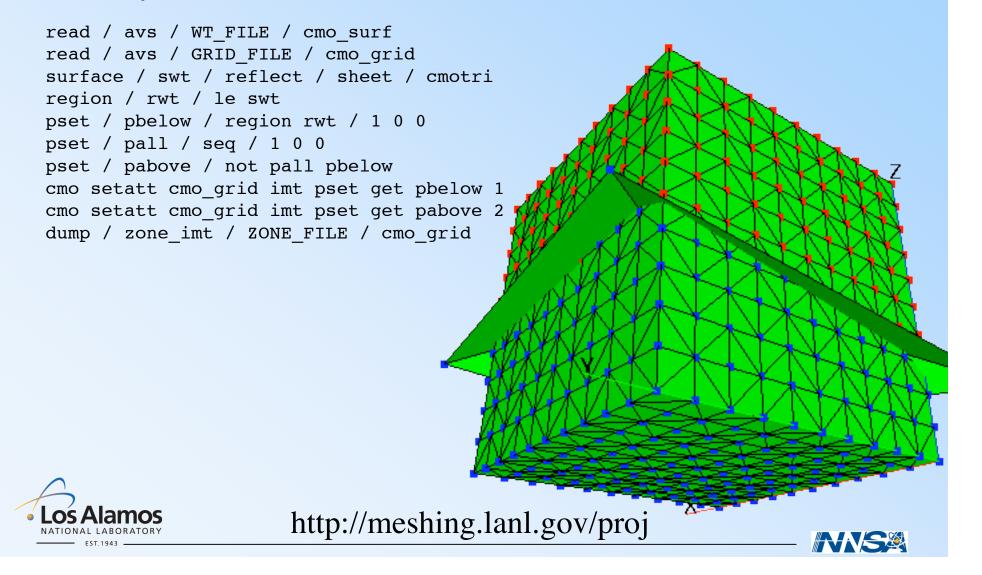


•Identify nodes above/below a surface (water table)

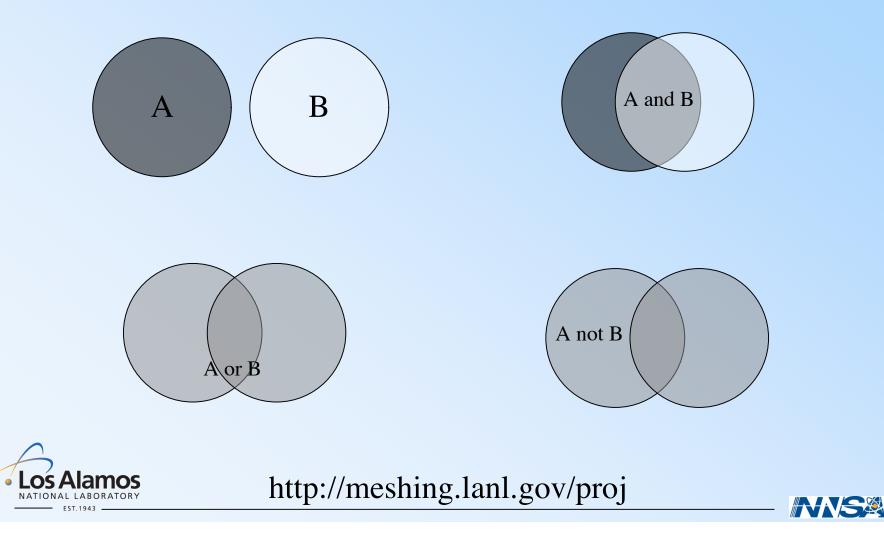




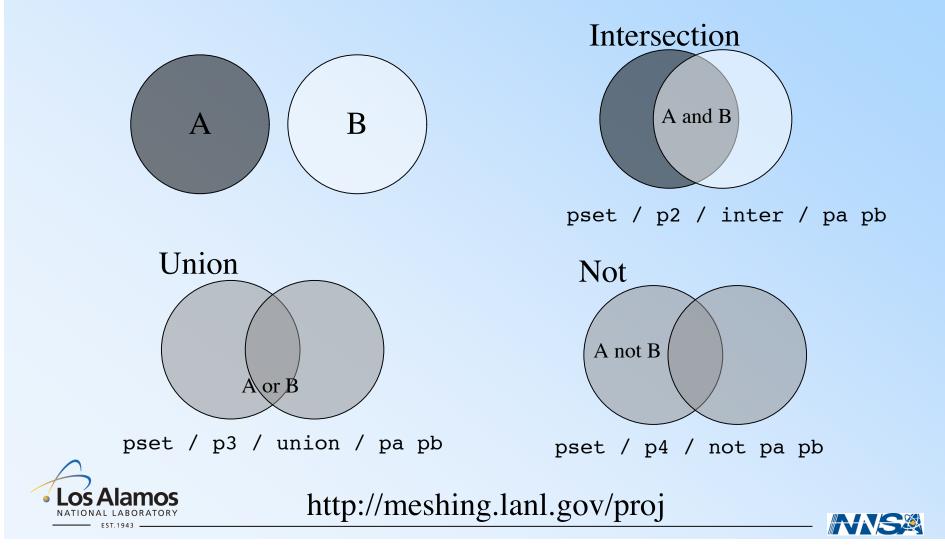
•Identify nodes above/below a surface (water table)



•Boolean operations on point sets (zone files)



•Boolean operations on point sets (zone files)



- •Boolean operations on point sets (zone files)
- •For Example:
 - •Nodes that belong to material_4 and are below the water table and are within 5 km of fault_5
 - •Nodes within 1 km of the topographic surface that are not within 1 km of a fault and are on the external boundary of the model





Meshing and Set Up Workflow

Problems and ChallengesAutomated (but not automatic)



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http://meshing.lanl.gov/proj

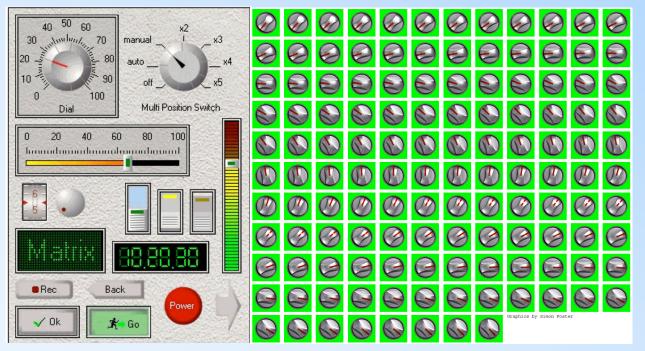
What users want.



Meshing and Set Up Workflow

Problems and Challenges

•Automated (but not automatic)



What users get.





No Silver Bullet

• A cookbook and the kitchen full of tools and ingredients does not make one a gourmet chef.

• What is required is a flexible tool kit and the expertise necessary to use the tools. One can then use expert knowledge to choose the right tool for the job depending upon the specific situation.



http://meshing.lanl.gov,1.01



Acknowledgements

- •Harold Trease
- •Lynn Trease
- •Denise George
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- Ahmed Khamayseh
- •Frank Ortega
- •Jan Wills

- Bob Walker
- Mike Murphy
- Rao Garimella
- Marc Witkowski
- Neil Carlson
- John Fowler





No Silver Bullet

 A cookbook ingredients

• What is req expertise ne expert knov job dependi







Meshing Non-manifold geometry

- Southern California Earthquake Center (SCEC) fault model for southern California
- 145 Faults defined by triangulated surfaces
- Surfaces have well defined normal (above and below surface) but since topology is not defined by closed volumes, a question such as, "Given an arbitrary location x,y,z, what material am I in?", is ill defined.

