Voxel-based finite element modelling with VOX-FE2

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Overview

Part I - Development of the VOX-FE2 plugin

- Finite element analysis and biomechanics
- Modelling voxel data
- VOX-FE2 and ParaView

Part II - The new VOX-FE2 solver and PetSc

Part III - A scheme for remodelling

Part I

Development of the VOX-FE2 plugin for ParaView

In this section

i. Finite element (FE) analysis
   - Application in biomechanical engineering

ii. Voxel data
   - Turning images into FE models

iii. Development of VOX-FE2
   - A brief history
   - Development as a ParaView plugin

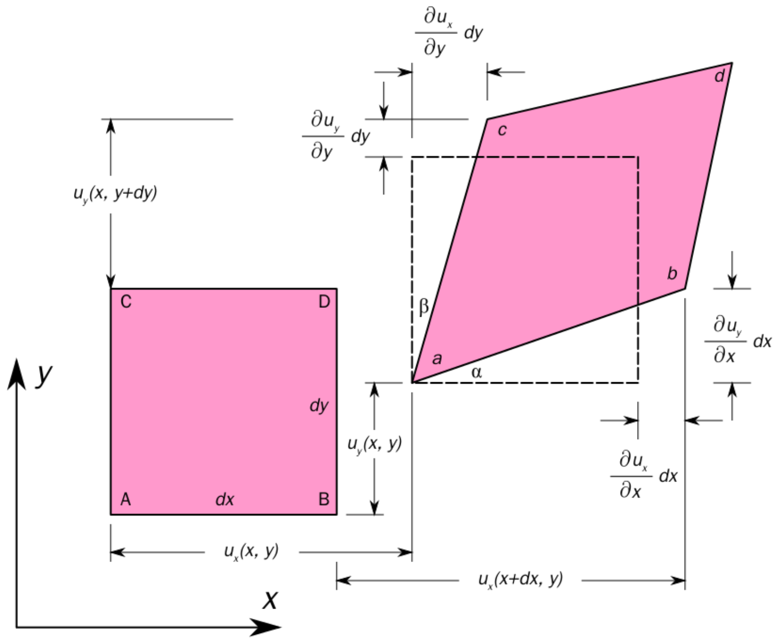
Finite Element Analysis (FEA)

- Well-proven and common place technique in engineering
- Becoming increasingly popular for the modelling of biological systems
- Used to calculate the deformation of any object when subjected to loads and to predict:-
  - Resultant stress and strain distributions
  - Reaction forces

FE in solid mechanics

FE treats the model as a series of much smaller elements

- For each element, we compute the distortion
  - Stretching (or squashing)
  - Shear
- The body is assumed to be elastic
  - For very small displacements



Sanpazderivative work: Mircalla22 (talk) - 2D_geometric_strain.png. Licensed under Public Domain via Wikimedia Commons

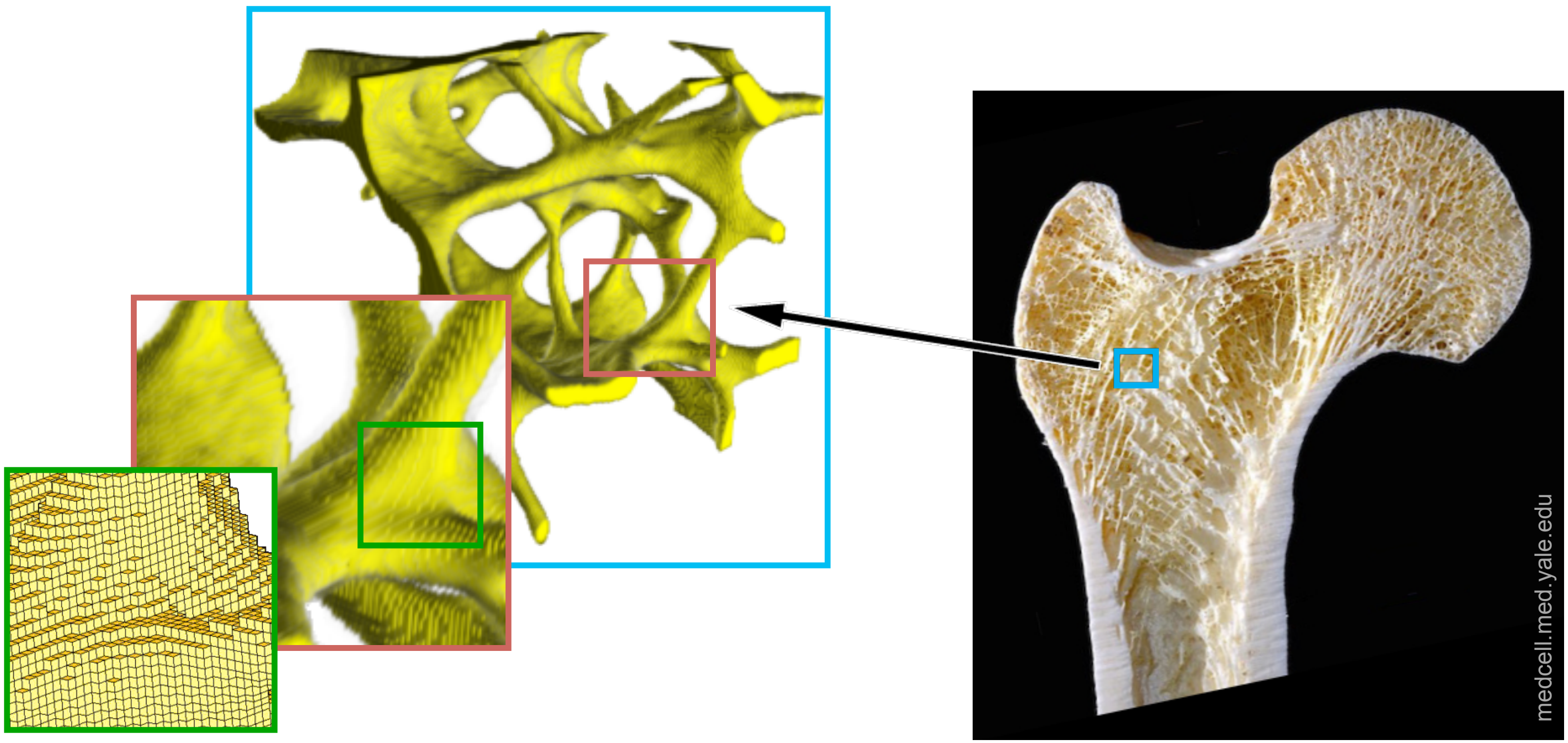
FEA in biomechanics

Bone is an obvious target for elastic modelling; but some form of simplification is usually required if current commercial software (eg. ANSYS or ABAQUS) is going to be used for analysis

- During that simplification, fine structures, especially trabeculae, may be lost
- Geometries are normally 'homogenized'
    - Elastic moduli are averaged over a small region, say
    - But, what happens near edges?
- Voxel-based modelling offers an alternative, multi-scale approach

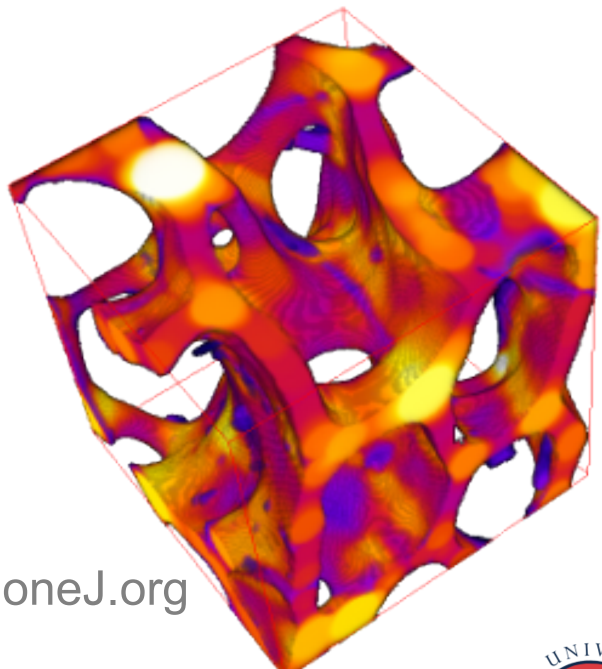
Voxel-based FEA

- Millions of voxels/elements needed to model small sections



How to set the resolution?

- A common metric is Trabecular Thickness (Tb.Th)
  - Largest diameter sphere contained within the model
  - Varies from species to species
- Some typical values for Tb.Th
  - 430μm Elephant
  - 134μm Human adult (F)
  - 20-60 μm Rodent
- For FE: working hypothesis
  - ≥ 5 voxels thick - 10 better !
  - cf Guldberg et al J Bio Eng 1998(120)



Source: BoneJ.org

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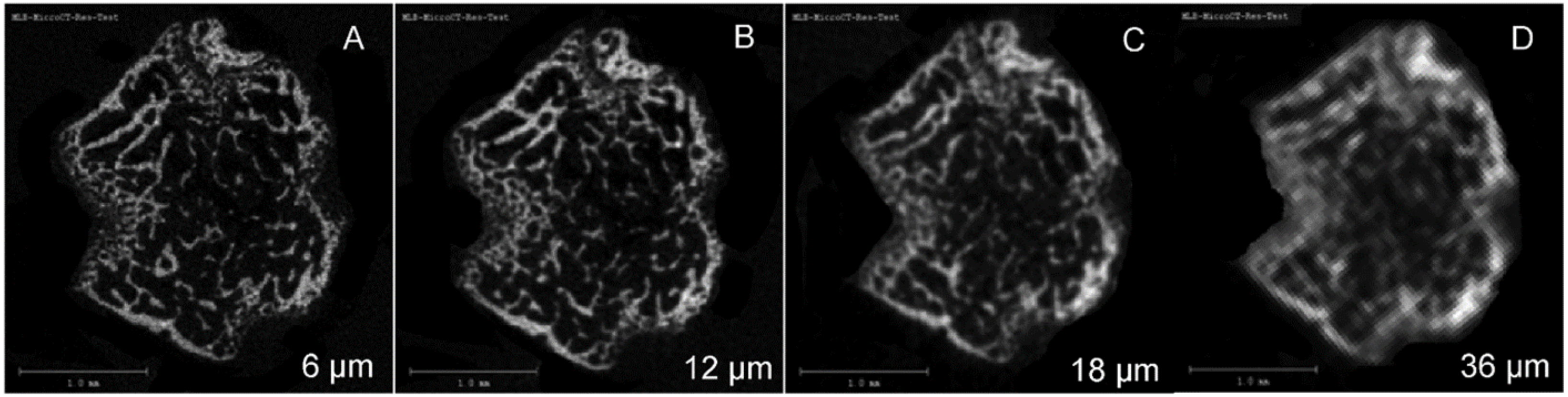
Example: MicroCT data (rodent)



Source: Bouxhein et al. J Bone Min Res 25(7): 1471

Besides resolution, for bone studies, we have to consider:-

- Nature of the problem
- Noise removal
- Image processing & segmentation

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Background to VOX-FE

Bone exists in a continual state of change

- Growth peaks in young adult life and after 35 years, begins to decrease
- At 70 years of age, more than 30% of the bone mass is lost
- Bone mass and structural morphology are affected by lack of exercise and disease

In 2003, Sisias established a framework for the investigation of remodelling with respect to:-

- Natural growth
- Metabolic disease (osteoporosis)
- External stimuli

The VOX-FE GUI

In 2009, in conjunction with Hull-York Medical School, a GUI was added

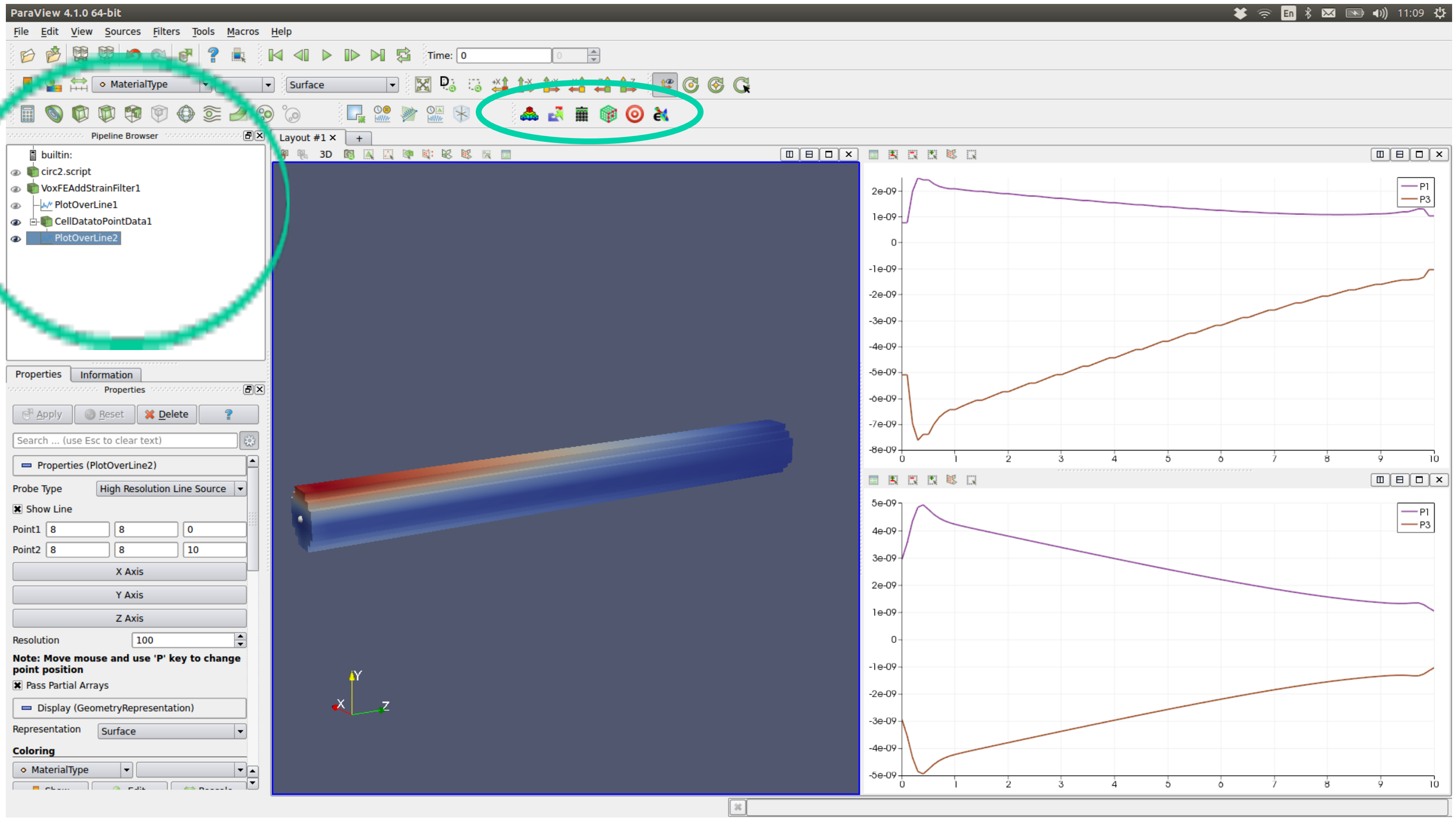
- Developed the script file format, for use with external solver
- Allowed display of boundary conditions, strains etc
- Optimised for voxel data

- Used Borland/Embarcadero C++ Builder (Windows)
  - Powerful RAD tool, but in retrospect, an unfortunate choice
  - No 64-bit version until recently (limiting to ~20M elements)
  - Relied upon graphics component developed by user community

ParaView

- Open source, cross-platform, 32 or 64-bit architecture
- Library of visualization tools, based upon Kitware's Visualization Toolkit (VTK)
    - A standard display model
    - Multiple views
    - Many filters already available
    - Undo/redo stack
- Well-documented pipeline-based interface
    - Tutorials, videos etc

ParaView/VOX-FE2 (example session)



Vox-FE2 plugin

Currently, the plugin has 6 main functions:-

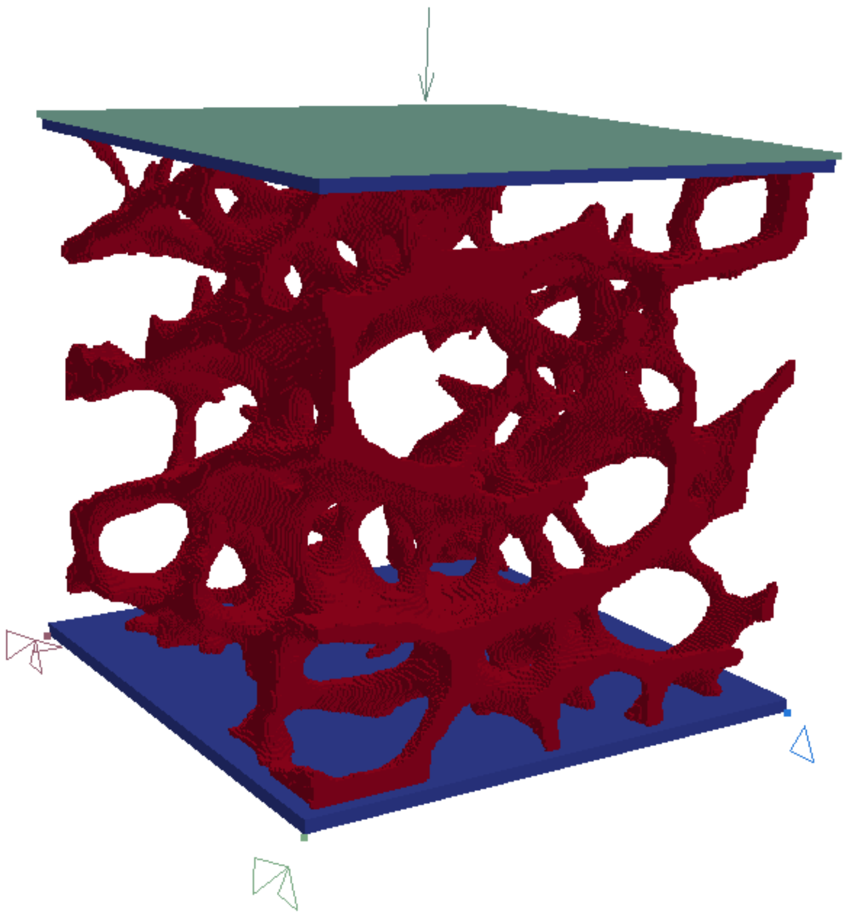
Pre-processing

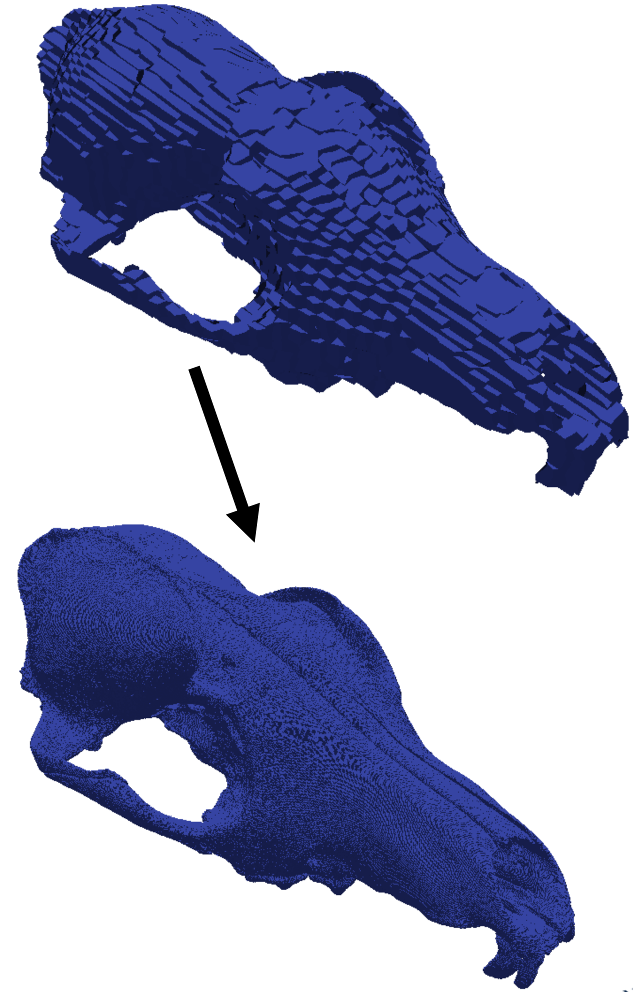
- Import/clean image data to create model (uses ITK)
- Group extraction (for ‘grouped’ data eg bone)
- Specify boundary conditions
- Display glyphs to illustrate boundary conditions
- Option to selectively export boundary conditions to a constraints file

Post-processing

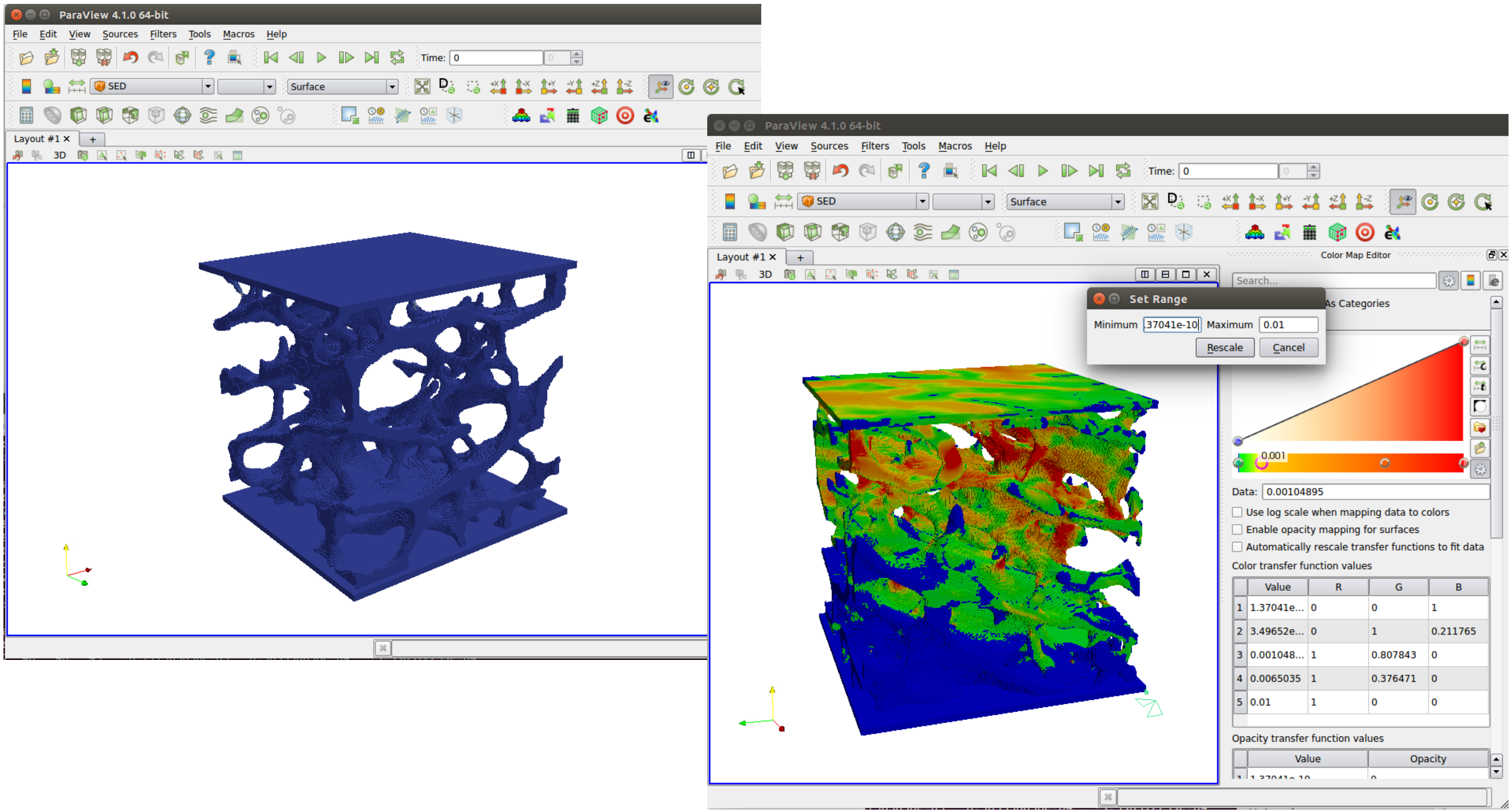
- Display of displacements, strains and stress

Glyphs/Level of detail operator





Colour-mapping strains



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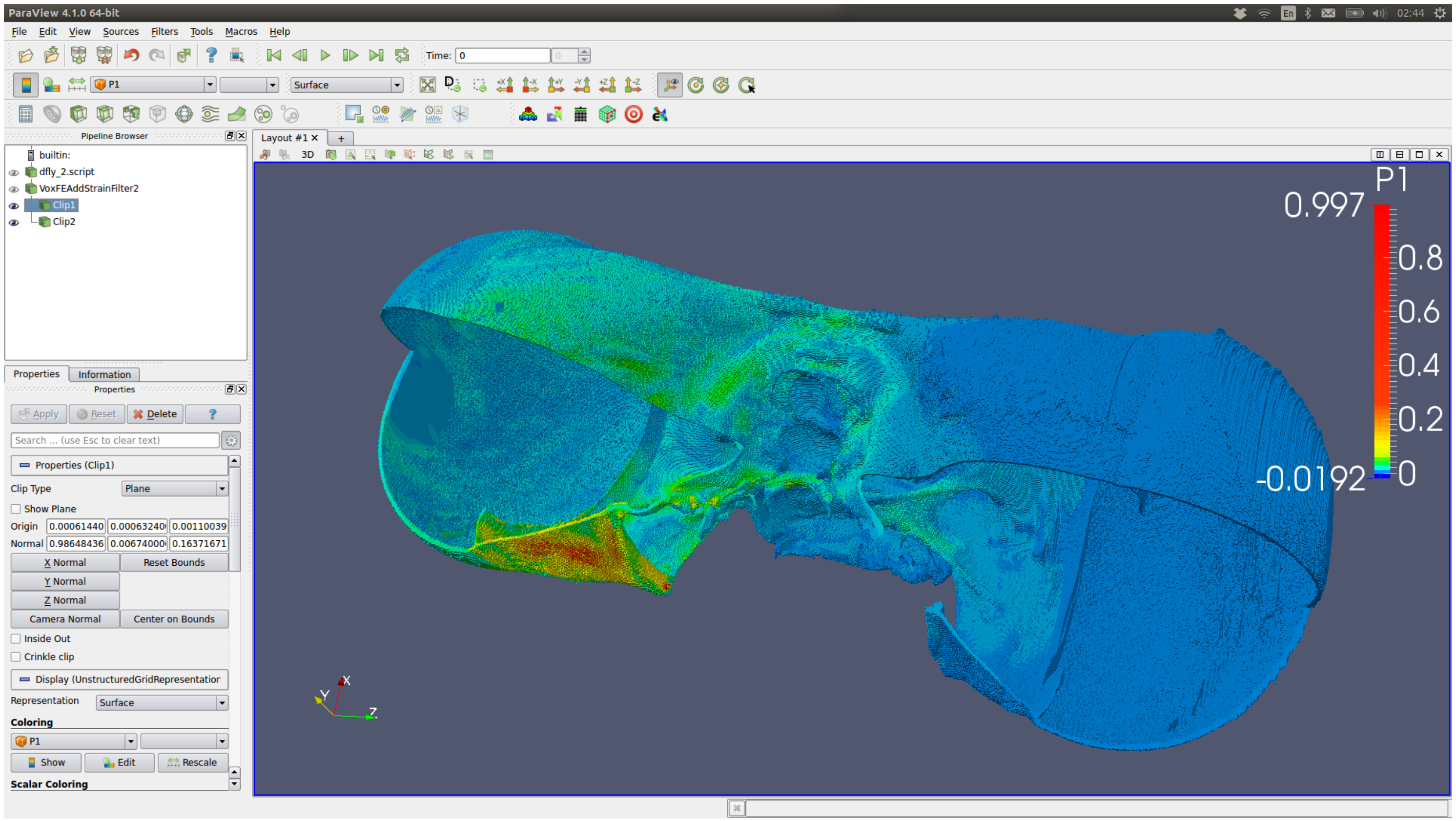
Clipping


ParaView 4.1.0 64-bit
File Edit View Sources Filters Tools Macros Help
Time: 0
P1
Surface
Pipeline Browser
builtin:
dfly_2.script
VoxFEAddStrainFilter2
Clip1
Clip2
Layout #1
3D
Properties
Information
Apply
Reset
Delete
Search ... (use Esc to clear text)
Properties (Clip1)
Clip Type
Plane
Show Plane
Origin
0.00061440
0.00063240
0.00110039
Normal
0.98648436
0.00674000
0.16371671
X Normal
Reset Bounds
Y Normal
Z Normal
Camera Normal
Center on Bounds
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Coloring
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Show
Edit
Rescale
Scalar Coloring
P1
0.997
0.8
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0.4
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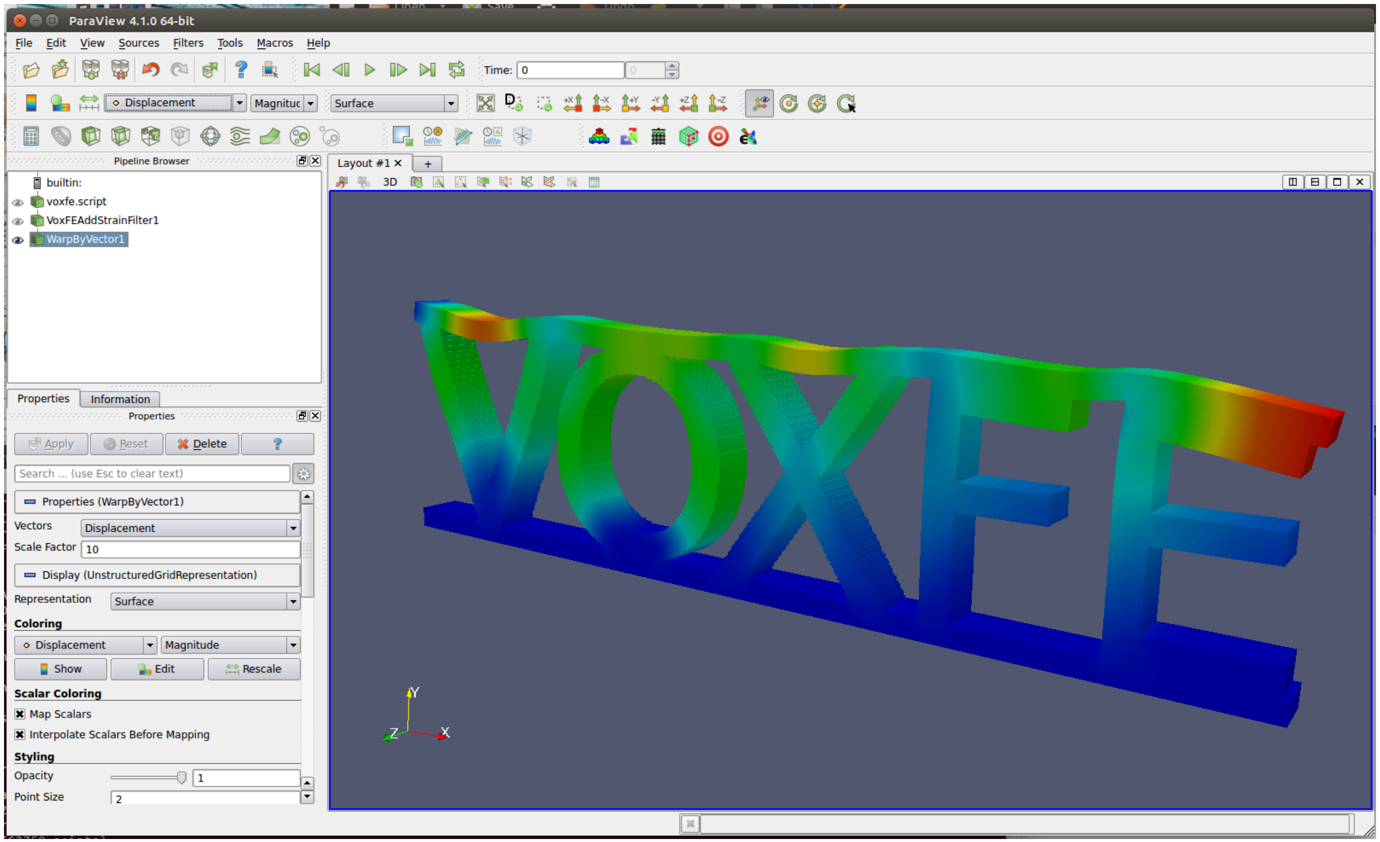
-0.0192
X
Y
Z

Adding displacement field



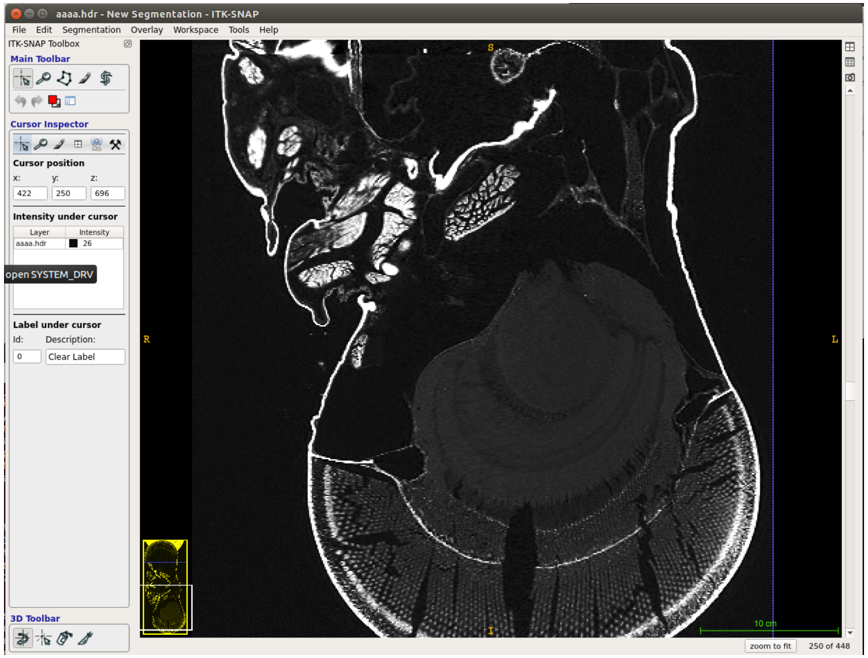
Summary

Now have much more stable, capable GUI

- Model exists as a standard VTK object
- ParaView incorporates many VTK filters
- Restricts the use of filters to the correct type for that object
  - Contouring, clipping, gradients, histograms etc
- Mutiple views, spreadsheets, 1-3D & animation
- 100M elements of desktop (32 GB RAM)
- VOX-FE2 plugin builds on Archer
- Expect to be able to using RSIP
  - http://www.archer.ac.uk/documentation/white-papers/rsip/ARCHER_wp_RSIP.pdf

Future work

- Features
  - Muscle-wrapping
  - Property definition based on grey scale
  - Examples & tutorials
- Modelling
  - MicroCT
  - Synchrotron data



Part II

The new VOX-FE2 solver

Solver : overview

- What the solver does
- Before VOX-FE2
- PETSc-based redesign of solver
- Performance results
- Summary

Solver : what does it do?

- Iteratively solves linear elastic problem

$$\mathbf{A}\,\underline{x} = \underline{f}$$

A Coefficient matrix

$\underline{x}$ Displacement vector

$\underline{f}$ Force vector

Solve using standard algorithms e.g. Conjugate Gradient Method

- **Challenge :** how to store and manipulate large matrices?
- For **10M** element model, **A** has ~O(10^{13}) entries of which **~0.0003%** are non-zero... **A** is **sparse**
- Find smart ways to store, manipulate non-zero values only

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Solver : before VOX-FE2

Optimised, parallel, linear solver written in C++, MPI

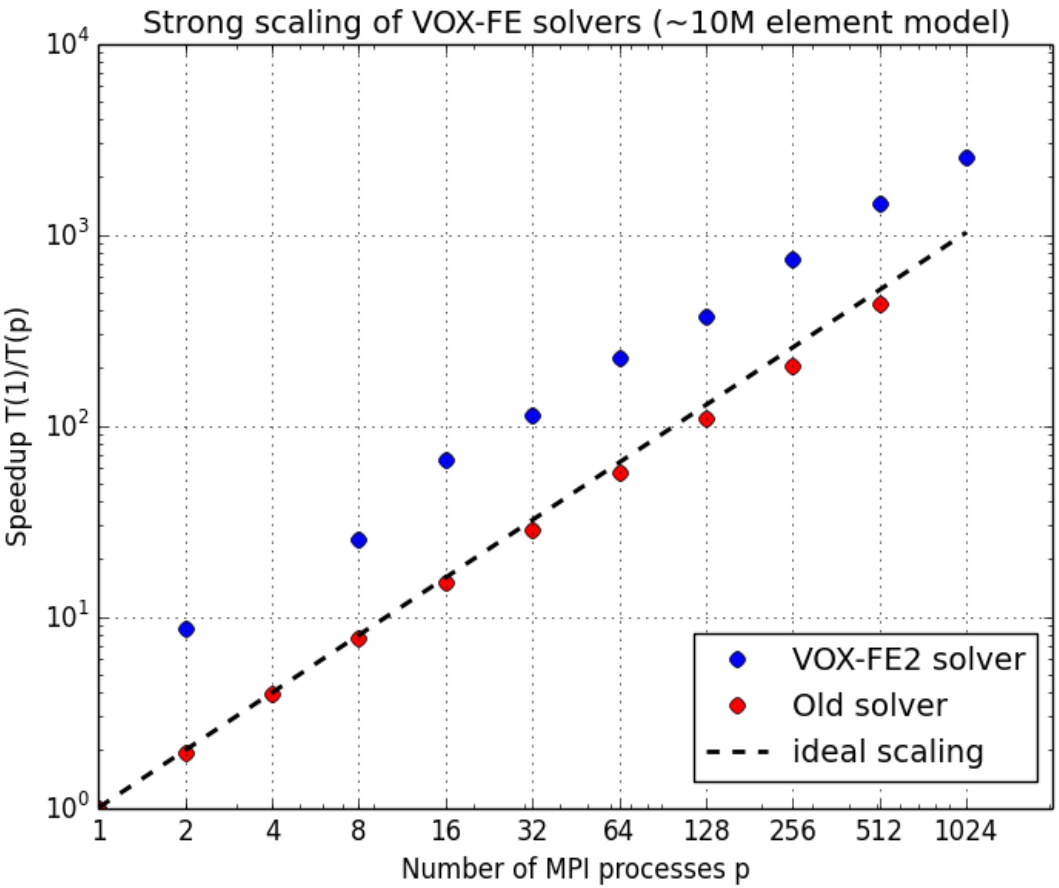
- Models up to 3 materials — **MORE MATERIALS**
- MPI partitioning along z-axis — **PARALLELISE ALL DIMENSIONS**
- Solves up to 20M elements — **LARGER MODELS**
- Scales well up to 256 cores — **MORE CORES, BETTER SCALING**

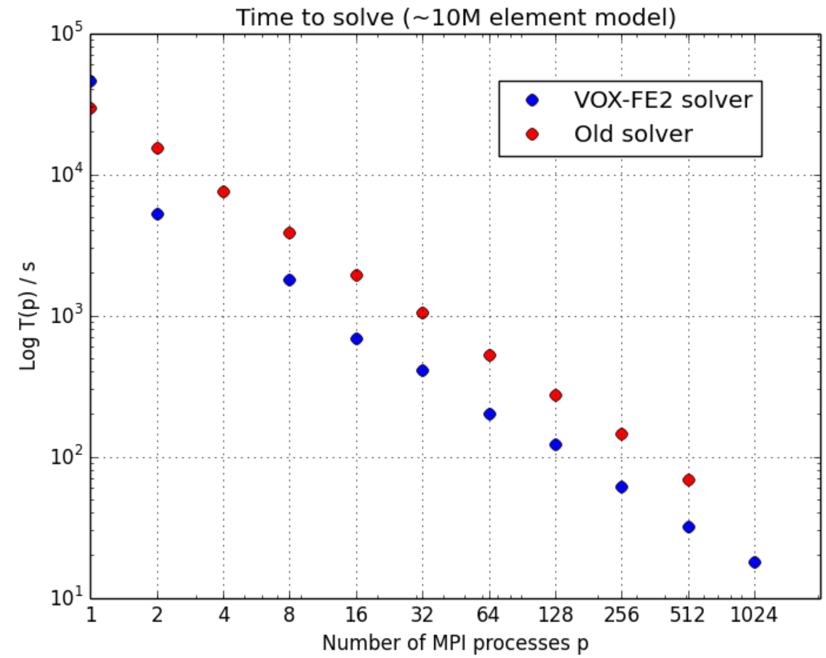
- Developer's $\$10^6$ question: extend code or start from scratch?
- Start from scratch because...
  - Difficult to implement **all the above** in old solver
  - There exist libraries that specialise in solving linear systems

Solver : PETSc-based redesign

- PETSc* is a library of data structures and routines for the scalable (parallel) solution of scientific applications
  *Argonne National Laboratory
- A PETSc-based solver has the potential to offer
  - Capability of running large models (~100M+ elements) efficiently with good parallel scaling along all dimensions
  - Greater choice of routines for solving the system, using different combinations of routines to get the best results
  - Fine tune PETSc to improve speed and scalability
  - Interface with ParMETIS for matrix/graph partitioning (remodelling)
  - Flexibility to run on heterogeneous architectures e.g. with GPUs

Solver : performance results





Solver : summary

In replacing old solver with an entirely new PETSc-based design, VOX-FE2 now has improved

- Scalability, speed, flexibility, extensibility, multi-material capability...

Future work

- Improve parallel decomposition using ParMETIS (currently solver splits matrix evenly between processors)

VOX-FE2 will be available on ARCHER and on Sourceforge (http://sourceforge.net/projects/vox-fe/) in the next few days!

Part III

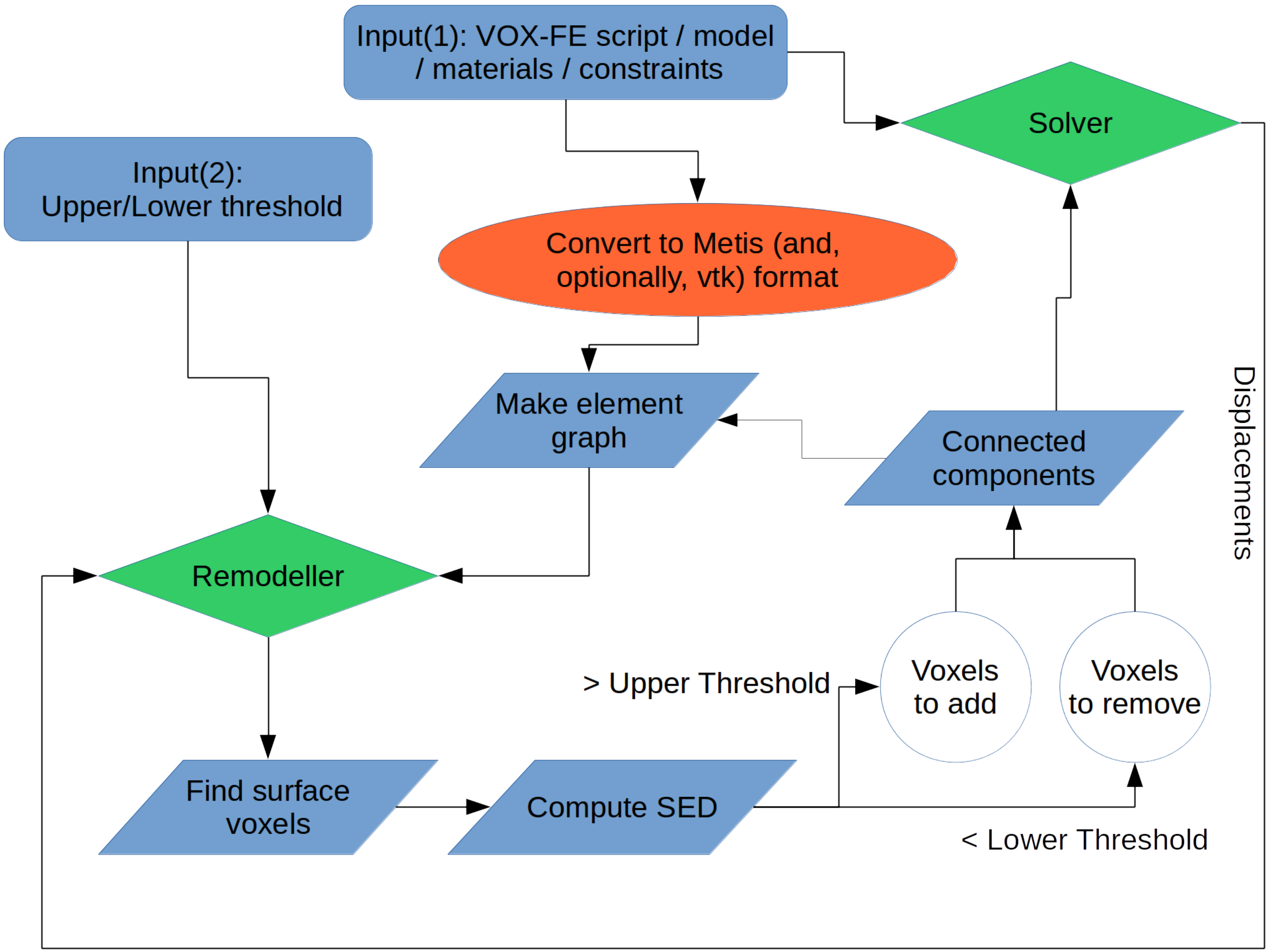
VOX-FE2:
A scheme for remodelling

Some concepts

- As observed earlier, bone:-
  - Exists in a state of flux resorption/growth
  - Age, disease and stress all have influence
- At this stage
  - Proving the concept
  - Naïve, can our models adapt to stress?
  - How can HPC help best?

Components needed

- Solver
  - Reads VOX-FE model data
  - Standalone (computes displacements)
- Organizing utility
  - Maintains a 'graph' of element connectivity
  - Computes strain data to add/delete elements
- Some form of 'glue' code


Input(1): VOX-FE script / model / materials / constraints
Solver
Input(2): Upper/Lower threshold
Convert to Metis (and, optionally, vtk) format
Make element graph
Connected components
Displacements
Remodeller
> Upper Threshold
Voxels to add
Voxels to remove
Find surface voxels
Compute SED
< Lower Threshold

Remodel/graph component

Reads in connectivity data from Metis

- Installed on Archer
  - Creates a very compact, but fixed graph
- VOX-FE Graph
  - Any voxel can only have 26 neighbours
  - Create bits for each neighbour (32-bit integer)
  - Easy search for surface voxels
  - 2-pass algorithm to remove disconnected elements (‘islands’)

Glue code

Working in batch mode:-

- Reuse GUI reader as offline utility,
    - convertVoxFEScript
    - m2gmetis
- Remodelling/graph component
    - Reads metis data and displacements
    - Reuse GUI strain component

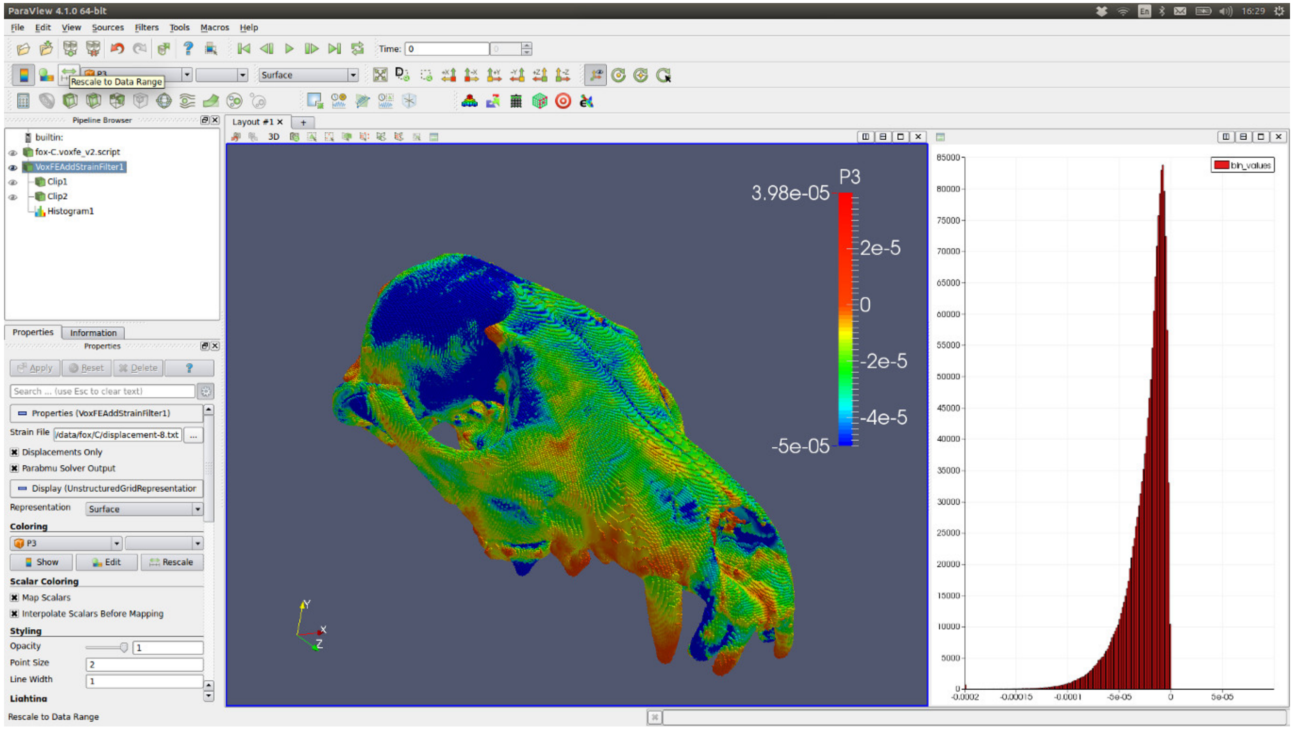
Scripts

Run remodelling from 2 scripts

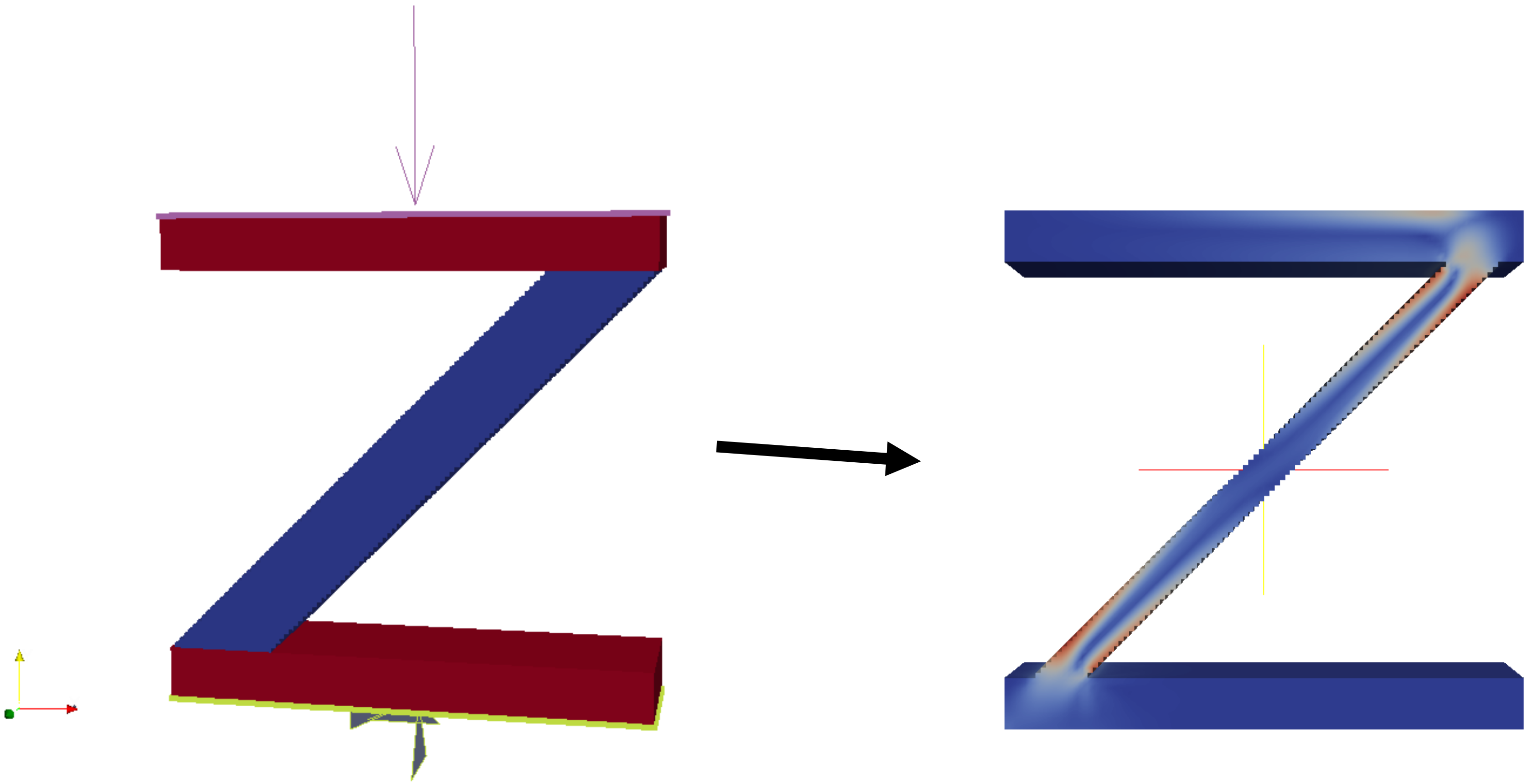
- Job submission launches ‘remodel’ script
    - Waits for solve to complete
- Once solver finished, waits for remodeling
- Currently, a new script/model file is created
- Process repeats until time or steps done

Choice of thresholds

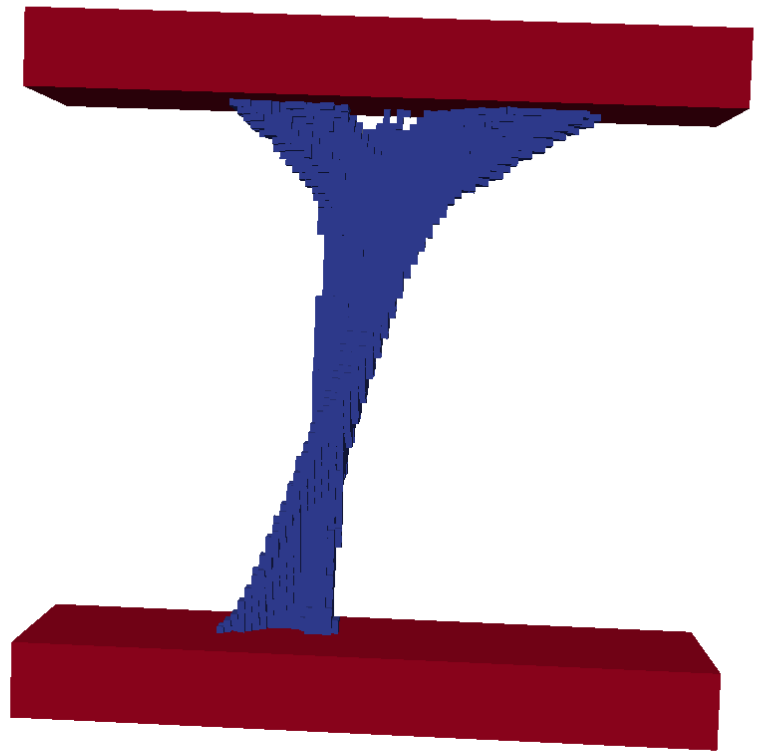
- Thresholds entered manually into job submission scripts
- Can be aided by first solve & histogram plot in ParaView



Example 1: ‘Z’ model



‘Z’ model → ‘I’



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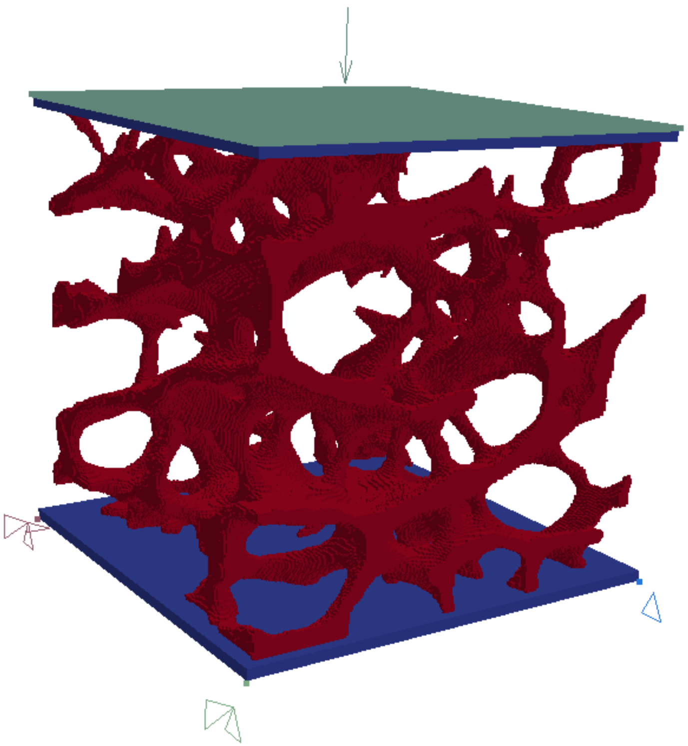
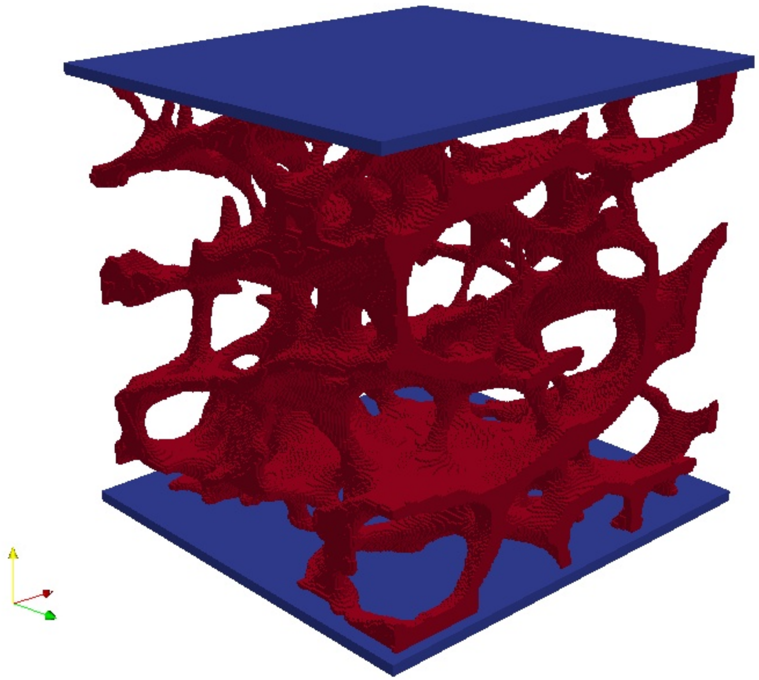
Example 2: Biomedtown ‘cube’



- Loaded evenly across top
- Based fixed
- Top/base cannot remodel

Remodelling in action (0)



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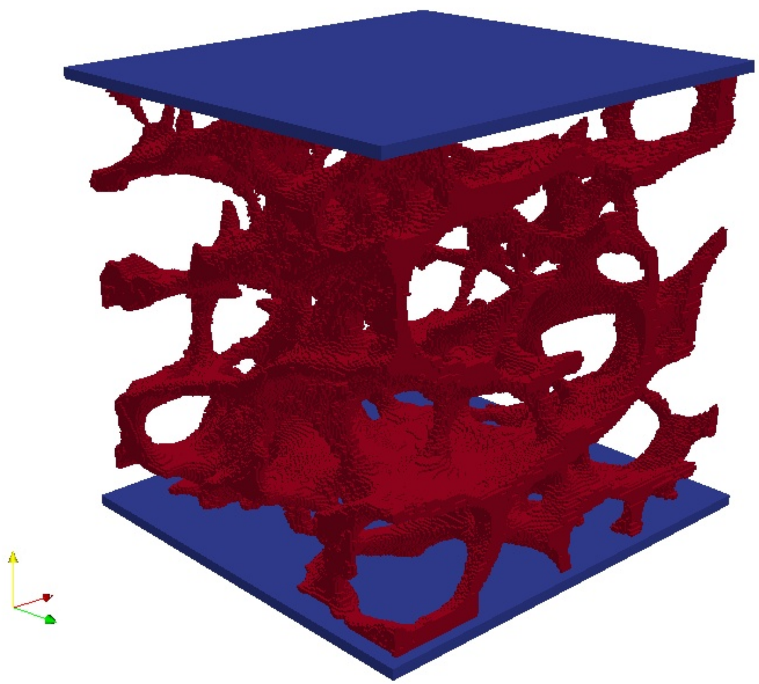
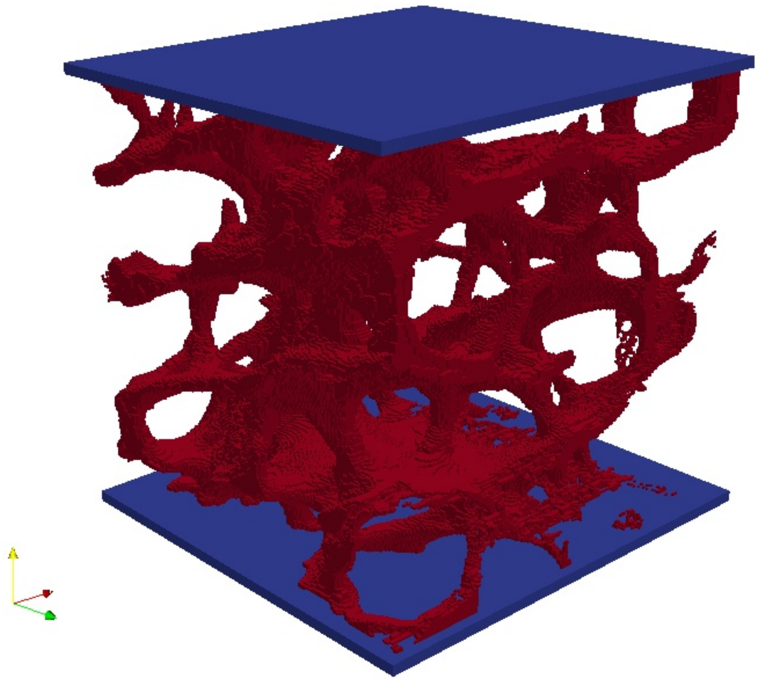
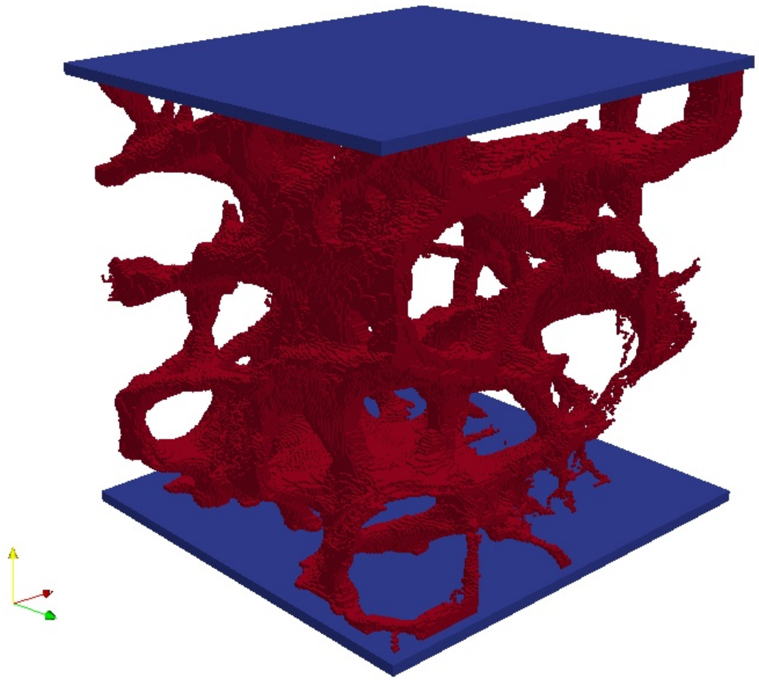
Remodelling in action (1)



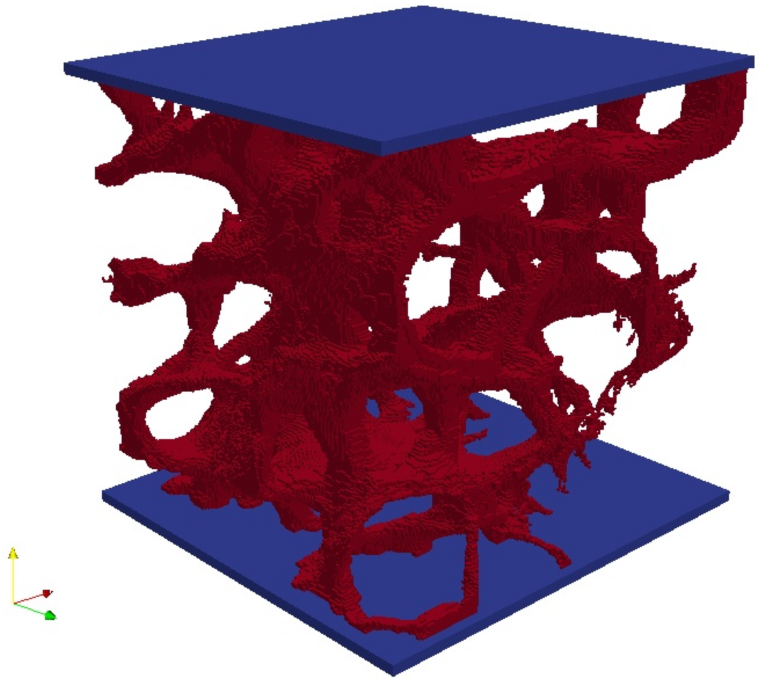
Remodelling in action (2)



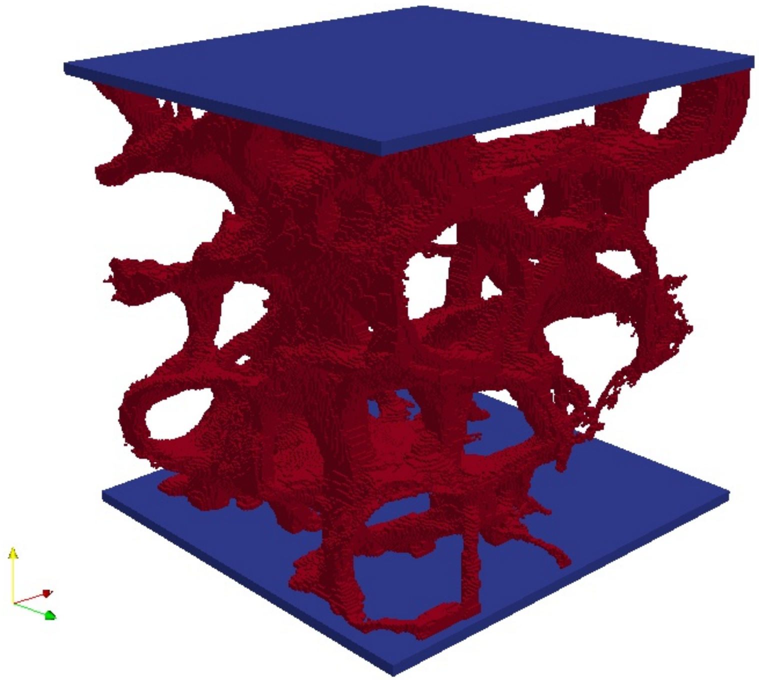
Remodelling in action (3)



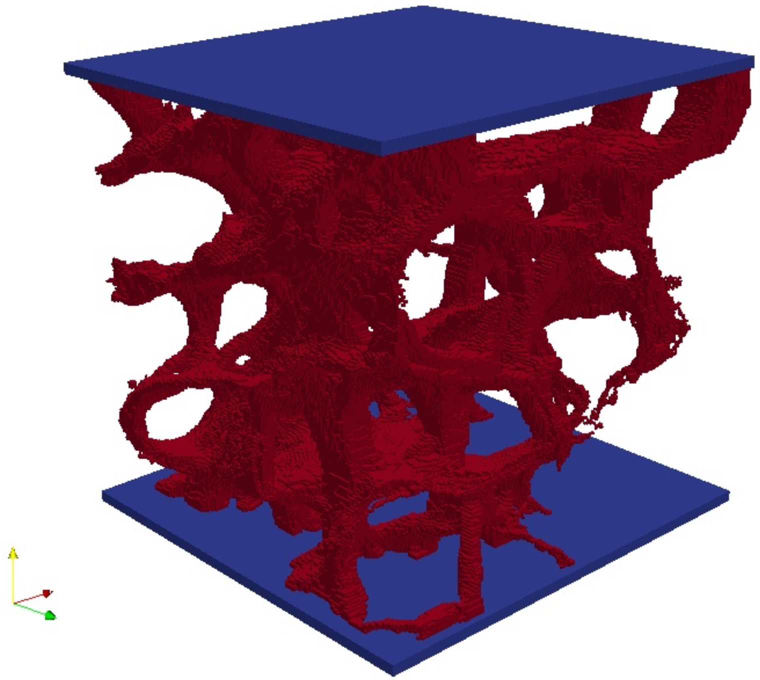
Remodelling in action (4)



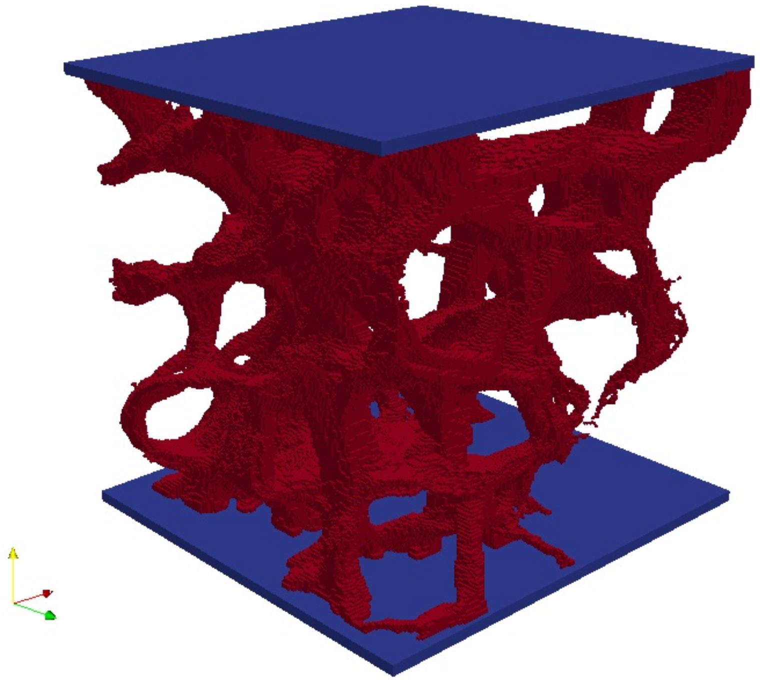
Remodelling in action (5)



Remodelling in action (6)



Remodelling in action (.)

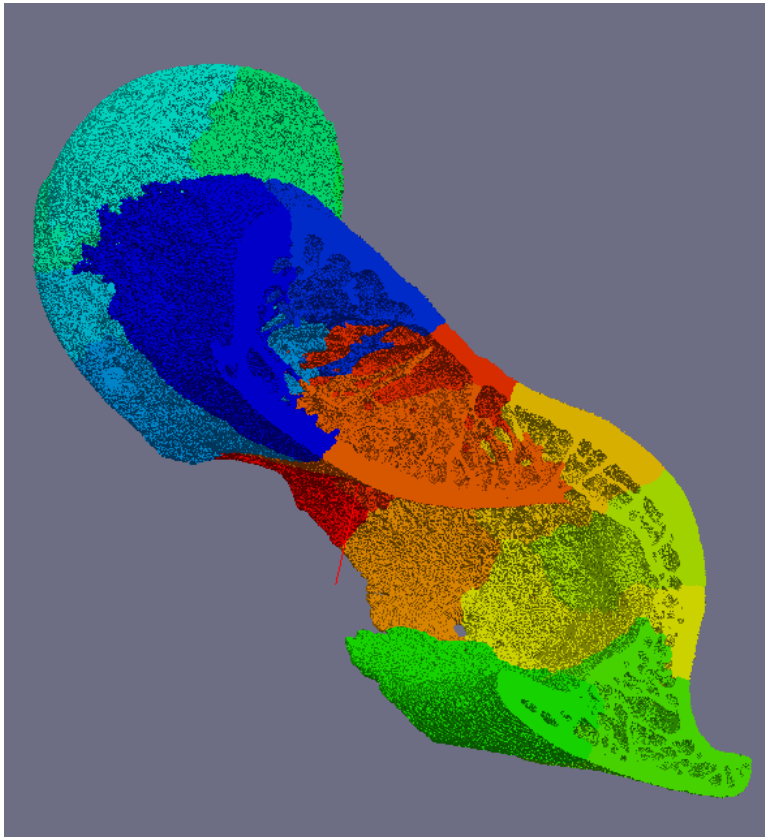


HPC

- 2M element trabecular model
  - solve 280 – 370s (16 cores, wallclock)
  - remodel < 10s
- Choice of thresholds problem
- Would prefer to solve in each dimension
- Larger models

Future work

- Adaptive remodelling
    - Statistical selected thresholds
- Graph partitioning scheme
    - (Par)Metis



Youtube video links:

Remodelling:

VOXFE: http://youtu.be/fjtjrM1Z1JQ

Biomedtown: http://youtu.be/WVp1u1jlD3g

'O' model: http://youtu.be/nT4xWlcm7aQ

Tutorial: http://youtu.be/DDeAxaZnE8U

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