

VOX-FE: New functionality for new communities

Neelofer Banglawala¹, Iain Bethune¹, Michael Fagan² and Richard Holbrey²

¹EPCC, The University of Edinburgh, ²The University of Hull

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1 Introduction

This report documents the work of ARCHER eCSE project 04-11 to improve and extend the VOX-FE finite element bone modelling suite. VOX-FE has been developed as in collaboration between EPCC and the University of Hull. VOX-FE consists of three parts:

- The graphical user interface - a ParaView plugin, which supports model construction from volumetric data (e.g. micro-CT image stacks), boundary condition definition (forces and constraints), and visualisation of strains and other derived properties computed by the solver. New functionality added to the GUI is outlined in Section 2.
- The solver - a parallel MPI application which given a model definition, constructs and solves the linear elasticity problem to compute the displacements of each node. A new model loading and load-balancing algorithm is described in Section 3.
- The remodeller - a scripting harness to couple together multiple executions of the solver to examine how bone adapts its structure under load. This process is now largely automatic, and is discussed in Section 4.

VOX-FE is freely available from <https://sourceforge.net/projects/vox-fe/> under a BSD license. The current released version is 2.0.1, and the next release 3.0 is planned pending the implementation of a parallel I/O method to enable the solver to produce correctly ordered output displacements (currently implemented as a post-processing script).

2 New Functionality in the VOX-FE GUI

2.1 Intensity Mapping

The VOX-FE plugin can read image data in several different forms (2D formats: jpeg, bmp, tiff, png and the 3D ITK mhd format). For later processing the image data are converted into script and model files, which can also be read directly by the plugin, to save re-importing later. Since version 2.0, the VOX-FE solver supports an arbitrary number of different ‘materials’ to be defined, enabling each imported voxel to have its own elastic moduli, rather than assuming it is uniform across all bone voxels.

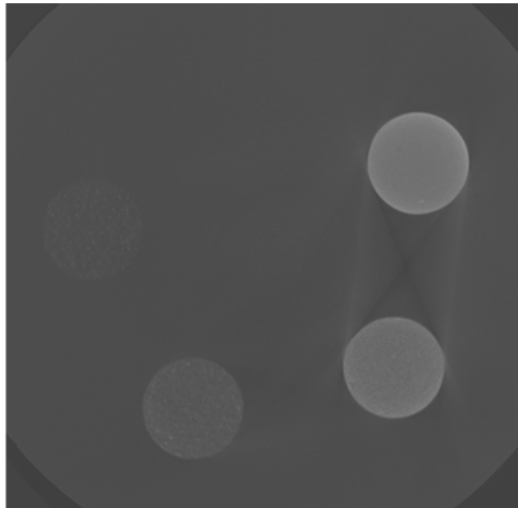


Figure 1: Example greyscale calibration samples

Raw intensity values (luminescence in grey-scale images) can be mapped to elastic moduli via an assessment of sample density, if phantom samples of known density are available to calibrate the CT machine (see Figure 1). A simple linear mapping between intensity and density can usually be assumed, but to compute elastic moduli from densities, the VOX-FE2 plugin implements a power mapping of the form presented by Carter and Hayes in 1977 [1] (quoted here from [2]), e.g.

$$\text{Elastic Modulus, } E = 3.79\epsilon^{0.06}\rho^3$$

where ϵ is the strain rate and ρ the apparent density.

In VOX-FE, we adopt the form:

$$E = A\rho^B + C$$

where A , B , C can be set in the filter dialog as the ‘Equation coefficients’.

2.2 Muscle-wrapping boundary conditions

Simple point boundary conditions are easy to apply within the GUI plugin: points are selected and the VOX-FE2 interface allows that data describing the load or axial constraint can be attached. Points within the same selection share the condition, so that separate BCs require different node selections. However, users would often like to model more realistic conditions such as the force applied by a muscle which is attached at specific points and wraps the bone structure, applying compressive forces on the surface. We have implemented the model of Grosse *et al* [3] which sets out a methodology to permit the modelling of muscle forces in terms of both tangential and compressive (normally-oriented) forces distributed over the area which the muscle is thought to be attached. In essence, this wrapping model views the compression of the bone as dependent upon 2 factors:

- the path length over which the muscle fibres are seen to be attached (the fibres become thicker and/or more numerous, so the load increases over the length of the path); and
- the curvature of the bone around which the muscle passes.

In short, the traction, $\tau(\vec{r})_N$, which compresses the surface can be described by the relation:

$$\tau(\vec{r})_N = s(\vec{r}) \cdot \kappa(\vec{r}) \cdot \tau(\vec{r})_T$$

where: $\tau(\vec{r})_N$ is the compressive load, $\tau(\vec{r})_T$ is the traction due to the intended action of the muscle (e.g. in biting), $s(\vec{r})$ is the length of the path of attached muscle and $\kappa(\vec{r})$ is the curvature of the bone attachment area.

Note that the authors have released a utility (BoneLoad) which can compute tangent and normal forces on tetrahedral meshes, but which requires a number of different utilities to run, including the commercial packages MatLab and Strand7.

Liu *et al* [4] have adapted this method for use with voxel data, using 2D splines placed by an alternate utility, which is interpolated across the mesh via a graph-based algorithm. A key difficulty is the mapping of the voxel surface to an approximation of the mesh surface: our approach is described below.

2.2.1 Surface Fitting

The muscle-wrapping algorithm of Grosse *et al* essentially requires that good estimates for curvature and the shortest geodesic path can be obtained on a given mesh surface. Unfortunately, for our voxel models, the surface is usually very coarse and assessments for these properties cannot be performed directly.

The first step is therefore to obtain a reasonable approximation of the voxel surface, for which we make use of ParaView to visualize the surface fit. As with the definition of point-based BCs, we rely upon the user to define the area of muscle attachment, which is then extracted.

2.2.2 Minimising Fitting Error

In order to minimise the error in fitting, these data are then transformed by principal components analysis (PCA), so that the axis of least variation is aligned with the z-axis of the PCA transformation, and becomes the axis over which the fit is performed.

One possibility is to use splines to perform this fit, but after experimentation with various open-source libraries (e.g. Netlibs surfits, and alglib), it was realized that the mesh approximation was still far too coarse. Another problem with these spline-fitting algorithms is that the fit must be retrieved on a regular grid, which would require further sampling to relate properties (curvature etc) back to the original grid.

An alternative approach, initially tested using the `fields` package in R, was to use `kriging`. This method has been developed by geologists using irregularly spaced samples to interpolate across any given region, and is therefore well suited to the problem of

irregular input samples. After further work, the `gstat` package in R was tried and it was found that on older C-version of the library also performed well for this purpose. This library has now been integrated into the VOX-FE plugin. (Eigen is used to obtain the PCA transform.)

2.2.3 Estimates for Normals and Curvature

ParaView (and the underlying VTK library) has several routines to assist with mesh construction and curvature estimation. It was found, however, that whilst VTK's `DeLaunay2D` filter provides a visually acceptable surface mesh approximation, used as an input to VTK's curvature estimator, the mesh gives poor results.

To improve the curvature estimation, several smoothing operators were tried (such as VTK's `vtkSmoothPolyDataFilter`) but with little success. A serious drawback to these methods is that they arbitrarily refine the mesh removing near coincident points. Whilst this presumably has great merit in terms of smoothing it also makes mapping back to the original points much more difficult.

Instead, a point-based method was slightly adapted from the code given in Dorias submission to the VTK Journal [5]. Since this method does not require an input mesh topology, and allows the radius of operation to be easily changed (giving a smoothing effect), it was much more readily integrated into the plugin.

A modification was added to the curvature estimator. Dorias code computed the average distance from the best fit plane to points within a sphere of given radius. This value was then normalized to lie in the interval $0 - 1$. Instead, we suppose that the average deviation, h , from the best-fit plane occurs at l (which is some fraction of the search radius L). A best-fit circle of radius r can then be found passing through this point and the centre of the search sphere. We define the angle a as:

$$a = \tan^{-1}(h/l)$$

By simple trigonometry, we know that the angle subtended at the centre of the fitted circle is $2a$. The search sphere (dotted in Figure 2) maps to a circle on the best-fit plane.

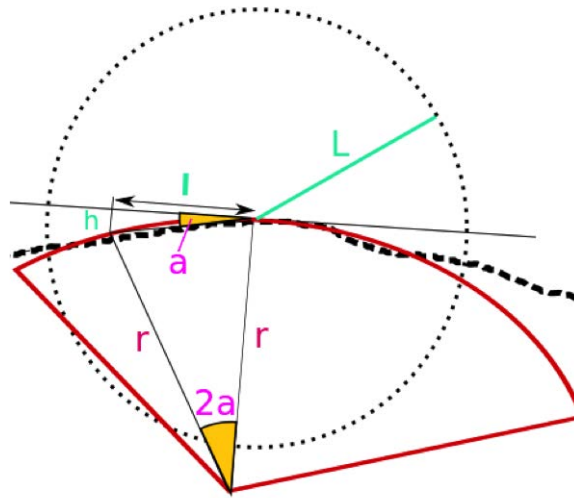


Figure 2: The modified best-fit circle algorithm

Assuming that the points within the search sphere are evenly distributed, then half of the points will fall within a radius $L/\sqrt{2}$ of the mapped circle (and half without). Thus, setting l to $L/\sqrt{2}$, we can estimate the radius r as:

$$r = (L/\sqrt{2})\cos^2(a)/\sin(2a)$$

This produces a clearer estimate of curvature ($= 1/r$) than the original code. Testing the approximation using `vtkSphereSource` meshes generated in ParaView typically yields values within 5% of the true radius.

The code for estimating normals works as given, provided that an outward orientation can be supplied. This can be readily computed from the PCA transformed point data, comparing data from the edge and central regions of the transformed space.

2.2.4 Computing the shortest path

VTK provides the `vtkDijkstraShortestPath` class to apply the associated shortest path algorithm on triangular mesh data. Using the Delaunay (2D) algorithm to compute the mesh topology, it is therefore possible to compute paths from each selected point

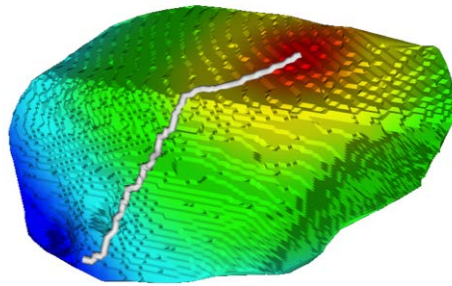


Figure 3: Shortest path between two points on the surface of a voxel mesh.

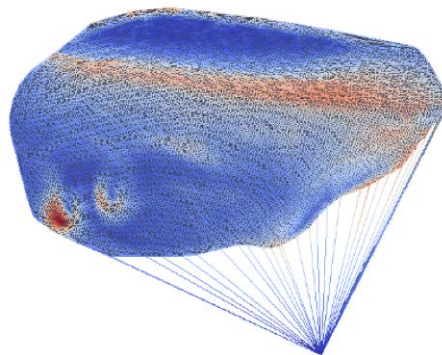


Figure 4: Concentration of paths towards a single point

towards a user-supplied target point (see Figure 3).

A problem occurs, however, where the mesh topology is constructed from the selected area towards the target point. A convex edge is established which minimises the number of triangles towards the target leading to an edge effect. This causes the paths to concentrate along a few strands towards the target point, rather than along possible grooves in the underlying bone (see Figure 4; note the surface colour mapping is by curvature).

To correct for this, an alternative graph algorithm was devised, using the Boost graph library¹. The Delaunay mesh can be interrogated to find the mesh triangles associated with the target point and neighbouring points are also recovered. The user is then requested to set a maximum edge side, say λ , so that all triangles with sides larger than λ

¹http://www.boost.org/doc/libs/1_61_0/libs/graph/doc/index.html

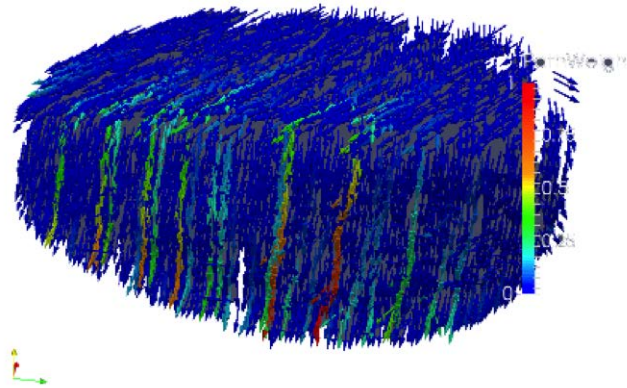


Figure 5: Distribution of strands along a path

can be removed and/or remodelled. This results in a much more even strand distribution, although there is still an accumulation along particular paths, see Figure 5.

2.2.5 Tangents

The Boost graph algorithm for the Dijkstra shortest path allows paths to be traced from every point to the target. Each point therefore has an associated path except where a path terminates. If this path segment is projected into the plane defined by the normal, then we can form the associated tangent. A resultant force can then be computed using the normal, tangent and curvature properties as described in Section 2.2.

2.2.6 Comments

The muscle-wrapping algorithm requires a number of properties to be defined which can be strongly affected by the choice of algorithm and the smoothness of the extracted surface. Time has not permitted the sensitivity of the algorithm to be determined for the factors obtained as described here. A further issue is the scaling of the normal (compressive) force which must be determined experimentally.

3 The VOX-FE 3.0 solver

3.1 Overview

The VOX-FE solver determines the effect of constraints and forces applied to a bone model. It does this by solving a system of coupled linear equations defined by a Global Stiffness Matrix (GSM), which describes the relationship between the bone elements making up the model and their material properties, and a force vector of any constraints placed upon the bone elements. Each bone element is a cuboid with eight nodes (the corners). When the linear system of equations is successfully solved, the solver outputs the final nodal displacements.

In eCSE01-15 [6], we developed VOX-FE 2.0, in which the legacy VOX-FE solver PARA-BMU was replaced with a PETSc²-based solver. The VOX-FE 2.0 solver (solver 2.0 from here on) outperformed the legacy solver in several ways: by solving larger models (> 20M elements) with an arbitrary number of material types, by scaling to higher core counts (> 256 cores), by being more memory efficient in using more cores per node and by offering a wider range of solution algorithms through the PETSc library.

In solver 2.0, every MPI process loads the whole bone model. This keeps MPI communication between processes to a minimum. However, it increases the memory cost per process as the model size increases. Construction of the GSM is divided evenly amongst processes, so that process p is responsible for the p^{th} set of consecutive GSM rows. The MPI communication involved in constructing the GSM and solving the linear system is handled by the PETSc library. For models with a dense, contiguous structure, e.g. a cylinder beam, dividing work between processes in this simple way works well. However, realistic bone models are sparse and have highly irregular complex structure which results in load imbalance across processors.

In this project we have addressed the load imbalance and memory efficiency issues of solver 2.0. We use ParMETIS³, an efficient, scalable graph partitioning library, to partition the model between processes so that work is balanced evenly across processes. We

²Portable, Extensible Toolkit for Scientific Computation [7]

³<http://glaros.dtc.umn.edu/gkhome/views/metis>

also introduce an improved method for model loading, whereby each process reads and owns a subset of the entire model. Thus the memory footprint of each process is reduced. These new developments are built into the VOX-FE 3.0 solver (solver 3.0 from here on) and are discussed in Section 3.2. The new solver's performance results, discussed in section 3.4, confirm that with good load balancing, it outperforms solver 2.0 for realistic bone models. Furthermore, the reduced per-process memory usage means that solver 3.0 is able to solve models an order of magnitude larger than the largest models solved with solver 2.0, and on a larger number of cores than was possible with solver 2.0.

3.2 Algorithm

The VOX-FE solver is written in C++ and parallelised with MPI. Figure 6 shows the main classes of the solver. The red highlighted methods are the key developments in solver 3.0.

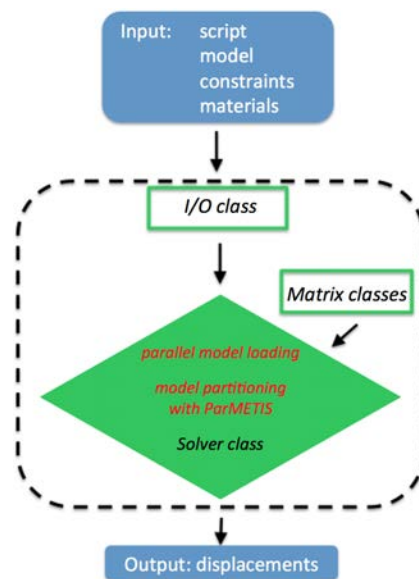


Figure 6: Solver 3.0: new developments are highlighted in red.

The overall algorithm for partitioning the model optimally is described below:

1. Model elements are evenly divided across processes.

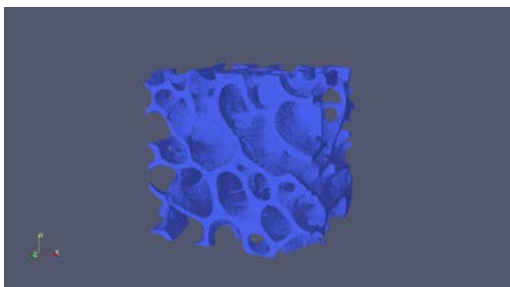
2. Each process has a set of local elements, `ElemS`, a set of corresponding local nodes, `NodeS`, a set of non-local or “ghost” (i.e. belonging to another process) elements, `GElemS`, and a set of corresponding non-local nodes, `GNodeS`. `GElemS` and `GNodeS` contain elements and nodes that neighbour the elements and nodes in `ElemS` and `NodeS` respectively. Note that it is necessary for every process to know all the neighbours of the nodes it owns (in `NodeSi`) in order to construct its part of the GSM: a GSM row corresponds to a node, and each non-zero GSM column corresponds to that node’s neighbour node(s).
3. Using the ParMETIS `Mesh2Dual` method, the element neighbours of each element in `ElemS` are found, which in turn determines the nodal neighbours of each node in `NodeS`.
4. Element and nodal neighbour information is distributed to all processes using `MPI_Alltoall`.
5. All nodes are renumbered so that each process owns a consecutively numbered set of nodes. This is necessary for using ParMETIS methods.
6. Using the ParMETIS `PartGeomKway` method, the optimal distribution of nodes across processors, i.e. the partition vector, is found.
7. Repartitioned element and nodal information is once again distributed to all processes using `MPI_Alltoall`.
8. All nodes are once again renumbered. This is necessary for the construction of the GSM, which requires that each node set is consecutively numbered.

Once the model has been partitioned, forces and constraints are loaded. The GSM is then constructed and the linear system is solved using PETSc. In solver 2.0, the final nodal displacements are sent to a master process that writes the displacements to a file in Cartesian order. In solver 3.0, to output the displacement data in order, it proved simplest to have each process write its set of nodal displacements to a separate file and then to collate the data in a single file using an external post-processing script. This is not an

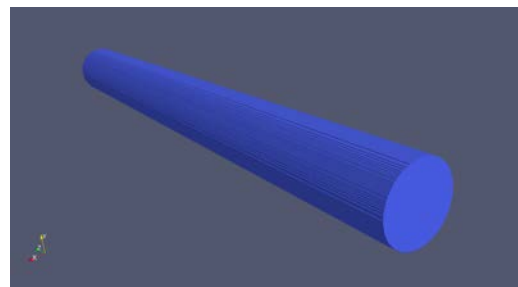
ideal solution but proved to be the most straightforward without requiring any MPI-IO methods or sending all the data to a master process which would cause memory issues when solving models with hundreds of millions of elements.

3.3 Test models

We tested the performance of the new solver using three different models: (a) a 200M element (sparse) horse bone cube model, (b) an 8M element (dense) cylinder model and (c) a 25M element (sparse) trabeculae cube model. Figure 7 shows models (a) and (b); model (c) is similar in structure to model (a). We chose these models to test the solver's performance on different bone geometries (idealised and realistic) and different sized models.



(a) Horse trabeculae cube model (200M).



(b) Dense cylinder model (8M)

Figure 7: Test models with total number of elements indicated in brackets.

3.4 Performance results

We ran all three models on solver 3.0. We also ran the cylinder model and the sparse trabecular model on solver 2.0; the horse bone model was too large for the old solver. Additionally, to maximise the per-core memory for the 25M element trabeculae model on solver 2.0, ARCHER nodes were underpopulated so that only one or two cores were used per node. Finally, we excluded the time taken to output nodal displacements from the performance data to make comparisons between the two solvers fairer.

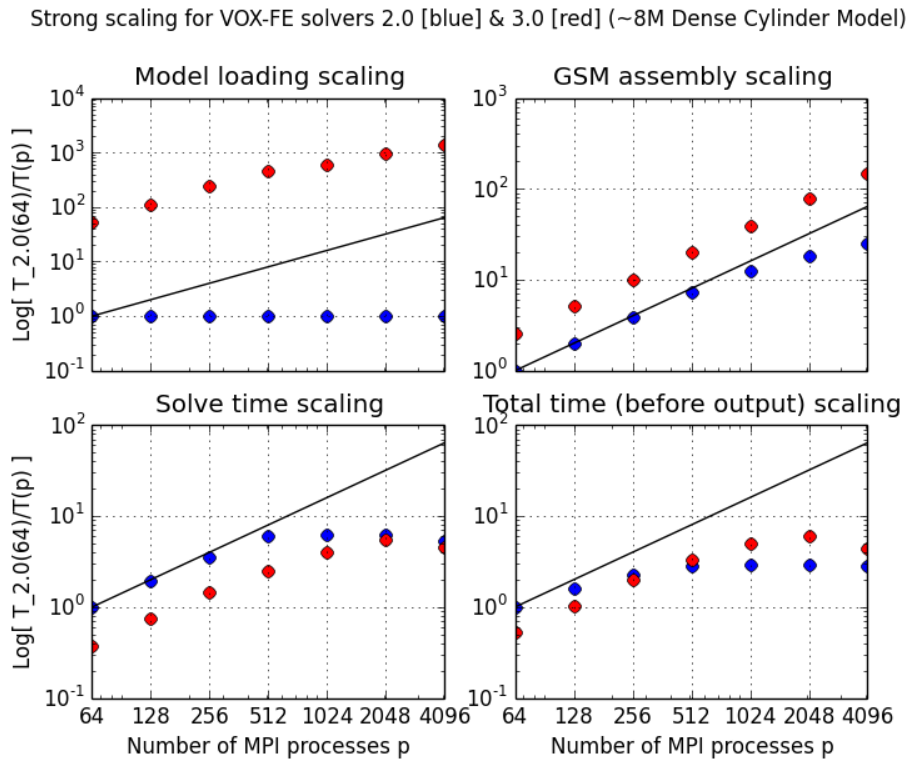


Figure 8: Strong scaling of solver 2.0 and solver 3.0 using the dense cylinder model (8M elements). $T(p)$ is the time taken by either solver on p processors and $T_{2.0}(64)$ is the baseline time taken by solver 2.0 on 64 processors.

Figures 8 and 9 show the strong scaling performance of solver 3.0 relative to solver 2.0. We see that the performance of the solvers varies between the two types of models. For model loading and constructing the GSM, solver 3.0 consistently shows super-linear scaling and outperforms solver 2.0. However, in solver 3.0, the time to solve the linear system scales sub-linearly for the cylinder model and drops below ideal scaling above 512 cores for the trabeculae model. The overall solver time for both solvers (excluding the time to output nodal displacements) scales sub-linearly in the case of the cylinder model, with solver 3.0 outperforming solver 2.0 on 512 or more cores. Solver 3.0 consistently outperforms solver 2.0 in the case of the trabeculae model, and shows super-linear scaling for up to 512 cores, before scaling sublinearly.

Figure 10 shows the strong scaling performance of solver 3.0 using the 200M element

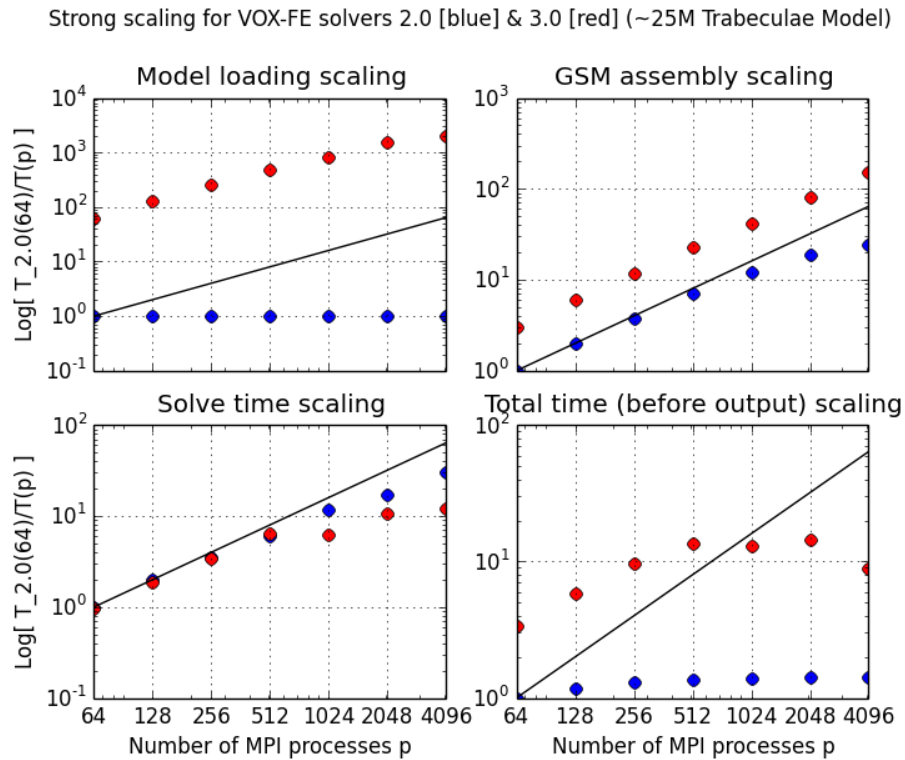


Figure 9: Strong scaling of solver 2.0 and solver 3.0 using the sparse trabecular model (25M elements). $T(p)$ is the time taken by either solver on p processors and $T_{2.0}(64)$ is the baseline time taken by solver 2.0 on 64 processors.

horse bone model. The solver shows close to ideal scaling up to 4096 cores.

3.5 Discussion

We have developed the next version of the VOX-FE solver, solver 3.0, by improving the overall load balance and the memory usage per core of previous solver. The performance results show that these developments have led to the solver now being able to handle models that are an order of magnitude larger than previously possible, and with good scaling on thousands of cores. Furthermore, the memory usage per core has been significantly reduced so that fewer nodes are needed to run the same model sizes on new solver compared to the old solver. This reduces computing costs and is more energy efficient.

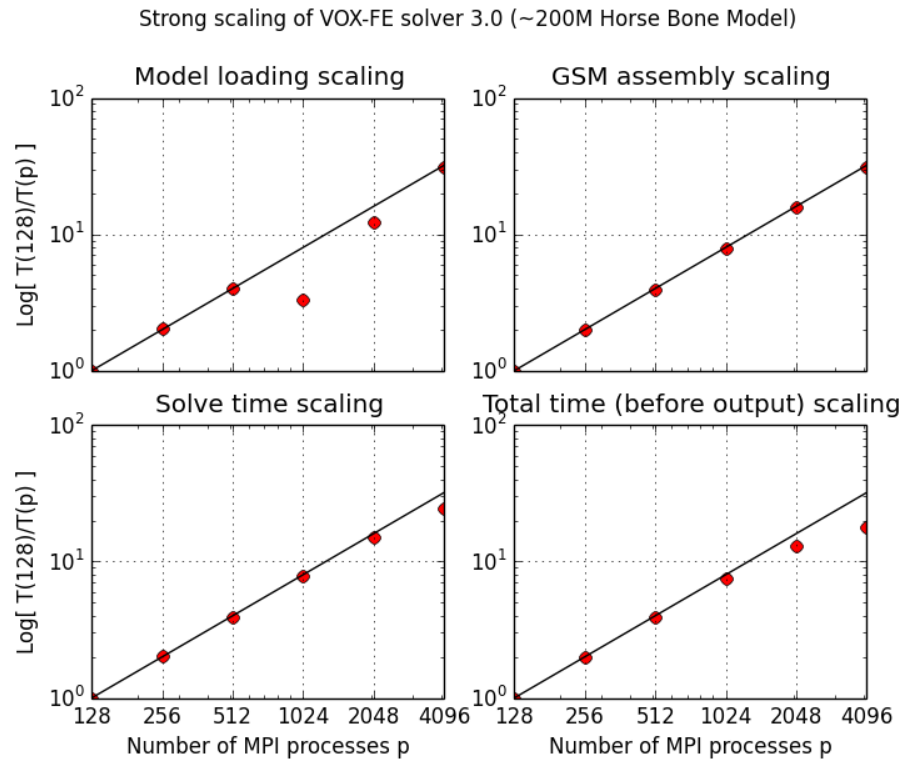


Figure 10: Strong scaling of solver 3.0 using the horse bone model (200M elements). $T(p)$ is the time taken by the solver on p processors.

Solver 3.0 performs well for realistic bone geometries. For smaller, less realistic models such as the dense cylinder model, ParMETIS may be unable to improve upon the simple model decomposition used in solver 2.0. Possible avenues for future work could include exploring why this might be and also how MPI-IO could be used to efficiently output the nodal displacement data to one file.

4 Adaptive Remodelling

An adaptive remodelling harness was added to VOX-FE in the 2.0 release, and is fully described in Section 4 of [6]. The main drawback of the initial remodeller was that selecting the upper and lower strain thresholds for applying remodelling was difficult, and the best values would vary from iteration to iteration as the structure adapted to the

imposed load and constraints. Two improvements have been implemented in this project:

- A formal command-line interface based on the Boost program options module, which can also be configured either on the command-line or by a simple text file; and
- An adaptive histogram-based scheme for the selection of thresholds.

4.1 Configuring the execution parameters

Running the help option of the graph control utility now yields the following output:-

```
>./voxfeRemodelControl --help
```

Generic options:

```
-v [ --version ]          print version string
-h [ --help ]            produce help message
-c [ --config ] arg (=remodel.cfg) name of configuration file.
```

Configuration options:

```
-i [ --script ] arg      VOX-FE script file
-m [ --materials ] arg  Binary file mapping ordered GlobalElementID to
                        MaterialID
-g [ --graph ] arg      Graph of node connectivity in element order
-a [ --adaptive ] arg (=Y) Use adaptive or hard threshold limits for adding
                        removing voxels. Enter Y/N
-l [ --lower ] arg      Lower threshold limit (enter value between
                        0.0-1.0 eg. 0.005)
-u [ --upper ] arg      Upper threshold limit (enter value between
                        0.0-1.0 eg. 0.95)
-k [ --lazycentre ] arg The lazy region (ie no further remodelling)
```

	centre, denoted K in the literature, typically $0.0025-0.005$
<code>-s [--lazywidth] arg</code>	The lazy region (ie no further remodelling) centre, denoted S in the literature, typically 0.3
<code>-z [--lazypop] arg</code>	When this fraction of the SED data is within the lazy region, remodelling will cease. Enter value between $0.0-1.0$
<code>-d [--displ] arg</code>	The name of the solver generated displacement file
<code>-p [--petsc] arg (=Y)</code>	Use the the PETSC-based solver, or the older solver (PARA_BMU). Enter Y/N
<code>-f [--fullconnec] arg (=N)</code>	Use full/26-neighbour connectivity to remove disconnected elements (aka islands), or the less drastic 6-neighbour connectivity. Enter Y for 26- or N for 6-connectivity

Note that whilst all the options presented can be given in a configuration file, particular options can be overwritten on the command line using the given tags. Thus to remind the user, the actual chosen command line options are stored in a generated file: `Remodelling.args.txt`.

4.2 Adaptive Remodelling

Using fixed thresholds has several drawbacks: finding good initial thresholds requires many runs to determine and often those starting values will give poor results after a handful of iterations. One factor, however, made the search for a more automatic threshold more awkward - namely that the range of SED values generated at the surface of models is neither normal nor half-normal. In fact, plotting histograms shows that the majority of the data lie in the first or the first few bins.

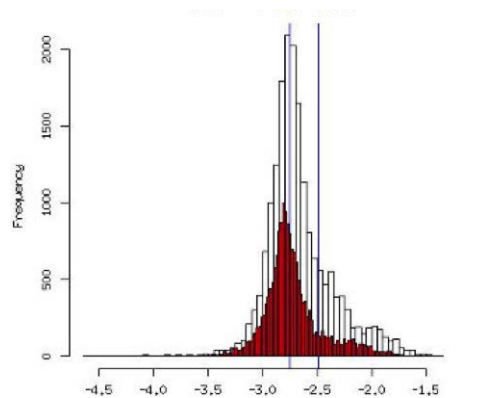


Figure 11: Example strain histogram, showing the effect of log scaling

The solution adopted in VOX-FE is to use a log scale to plot the histogram. Although no longer a true histogram, this shows a much more normal shape, which is more amenable to the selection of upper and lower populations (see Figure 11). If the user selects adaptive thresholding (see Section 4.1), then two other parameters must be provided giving the fraction of the population below which voxels are removed and that fraction of the population above which voxels are added. Since more voxels tend to be added than removed, it is advisable to set these to be uneven e.g. 0.05 and 0.995.

Weinans *et al* [8] and several others have proposed that a ‘lazy zone’ can be defined in which no further growth should occur. A zone (centre [-k] and width [-s]) can be set in the configuration file which will terminate the remodelling process if a sufficient percentage of the population should be found to lie within this zone.

4.3 Discussion

The process outlined above could be streamlined, particularly with regard to (re-)reading input files. Ideally, the graph control would remain resident throughout, checking periodically for the generation of appropriate files, perhaps, via notifications from the solver through a socket interface. The current scheme, however, has the advantage of simplicity and ease of debugging as all intermediate files are available.

Although use of the connected components algorithm is advised to remove separated

bone ‘islands’, the solver has so far proved to be robust to models with small numbers of disconnected elements. Possibly this is because such regions are generally well away from regions of high strain, so that the impact is slight. The less severe 26-face check is therefore favoured currently, but it should be noted that only the 6-face connectivity option removes all weakly linked (i.e. node or edge only) element connections.

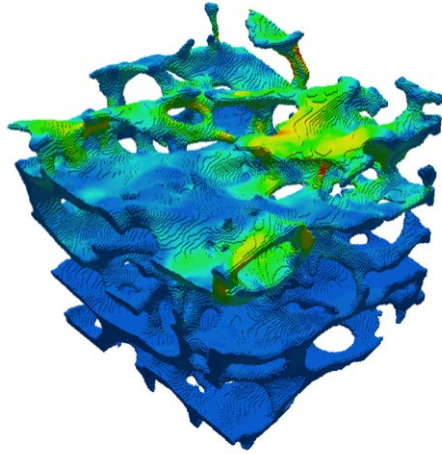


Figure 12: Strain energy density visualisation of a trabecular bone model. Yellow and red indicate regions of high strain, where new voxels will be added prior to the next remodelling iteration.

Due to some memory issues with the 2.0 solver, only models of around 2 million elements have been tested within the above scheme. The wall-clock time for this solving the model, shown in Figure 12, lies between 280-370 seconds (on 16 cores), with the remodelling step requiring less than 10 seconds.

Setting the ‘lazy zone’ to terminate the remodelling process, which should lie around 0.0025-0.0052 J/g ($\pm 30\%$) according to the literature, has not proved to be very workable so far. It is unclear if these values may be too restrictive or whether these values may vary for different bone types. Given that the zone is now highly configurable in VOX-FE, however, it should be possible, with further experimentation, to define a likely termination zones.

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