ARCHER CHAMPIONS
OXFORD

5TH - 6TH SEPTEMBER 2016

VOX-FE
A tale of two eCSEs

Neelofer Banglawala, Iain Bethune (EPCC)
Michael Fagan, Richard Holbrey (University of Hull)

Overview

- Background

- eCSE-01 – large scale voxel based modelling
  - VOX-FE 2.0

- eCSE-04 – new functionality for new communities
 - VOX-FE 3.0

- eCSE outcomes

- Summary

Background : bones

- Bone exists in a continual state of change
  - Bone remodelling via resorption and ossification
  - Peak growth in young adult life. Bone loss begins after age 35. By age 70, more than 30% of bone mass lost
  - Lack of exercise and disease cause loss and structural changes
- Bone is made up of different types of materials and has complex geometry
- How does bone respond to forces and constraints?
  - difficult to investigate this *in vivo*
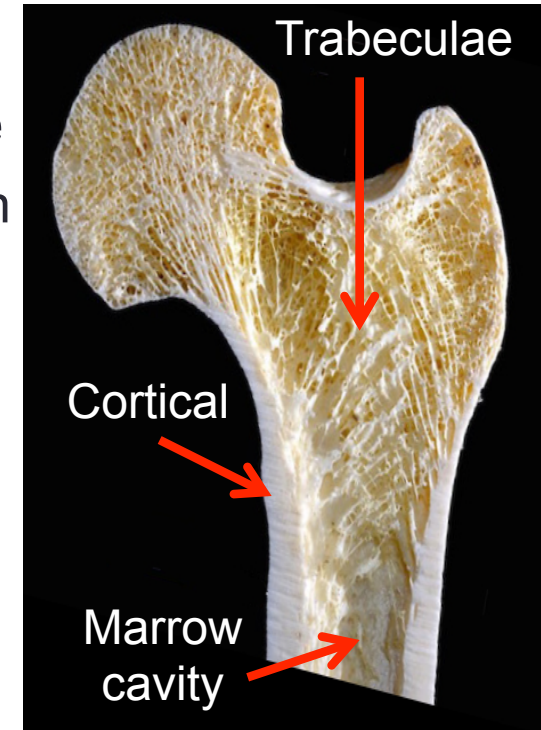
Background : bones (cont.)


medcell.med.yale.edu

- Model bone as made up of millions of small cubic elements called voxels (finite elements)
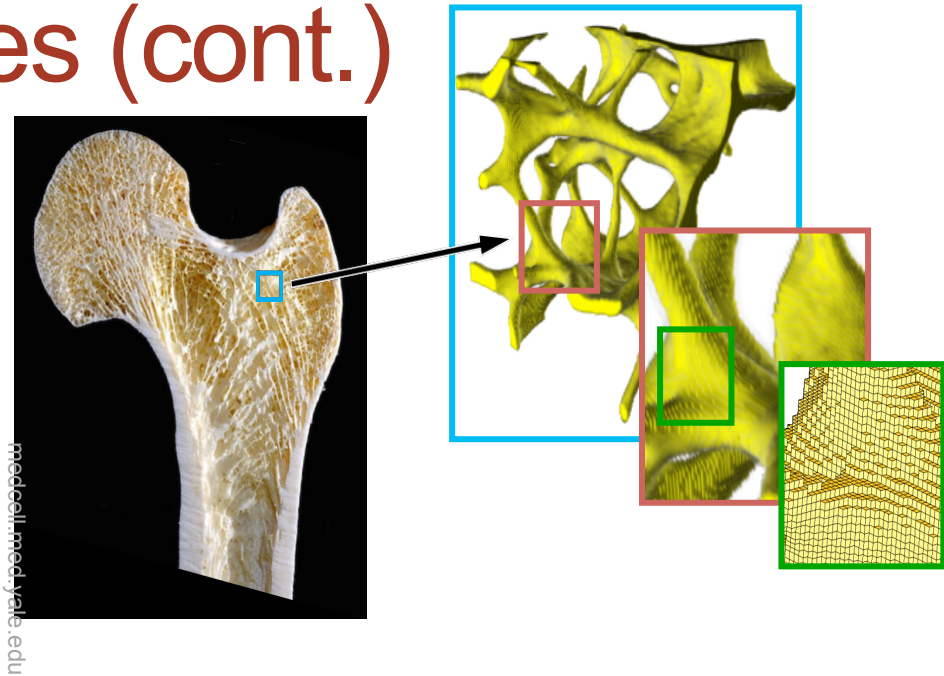
- **VOX-FE** is a voxel-based finite element software suite for the analysis of bone models
  - Developed jointly by Michael Fagan's Medical & Biological Engineering (University of Hull), Hull-York Medical School and EPCC
  - Consists of frontend GUI and backend linear solver

Background : legacy VOX-FE

- Prior to eCSE development work, VOX-FE could
  - handle models of ~20 million elements, max 4 material types
  - good scaling up to ~256 cores
- But for realistic bone modelling, need
  - to handle large, complex models of several hundred million (billion?) elements, arbitrary number of materials ...
  - good scaling to thousands (plus) cores in order to run large models on HPC capabilities
- Also want to investigate remodelling process, effect of muscle wrapping and much more...
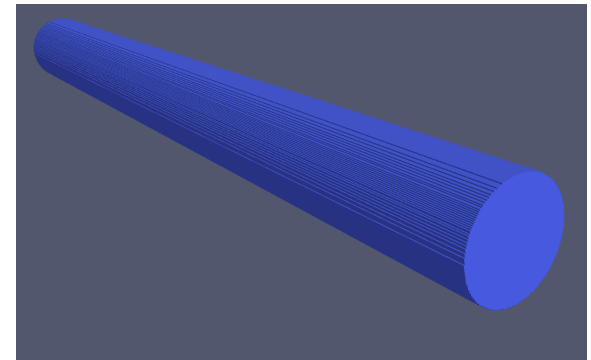
eCSE-01 : VOX-FE 2.0

- Large scale voxel-based modelling
  - April 2014 to April 2015
  - Hull: Michael Fagan (PI), Richard Holbrey (tech)
  - EPCC: Iain Bethune (Co-PI), Neelofer Banglawala (tech)
- 15 PMs split between EPCC (7 PMs) and Hull (8 PMs)
  - WP1 – Develop PETSc-based linear solver to replace old solver
  - WP2 – Support for multi material-type models in the PETSc solver
  - WP3 – Initial implementation of adaptive remodelling
  - WP4 – GUI redevelopment with ParaView plugin for large models
- Travel budget for 2 face-to-face meetings

eCSE-04 : VOX-FE 3.0

- New functionality for new communities
  - e.g. palaeobiology community, for reconstruction of fossils
  - April 2015 to Feb 2016
- 9 PMs split between EPCC (3 PMs) and Hull (6 PMs)
  - WP1   – Solver improvements - load balancing with ParMETIS
  - WP2-4   – Muscle wrapping, self-tuning remodelling (and improved material definition mapping from CT image scan)
  - WP5   – Open source release (including user guide and tutorials)
- No face-to-face meetings – work packages assigned to either either EPCC or Hull

eCSE : Outcomes

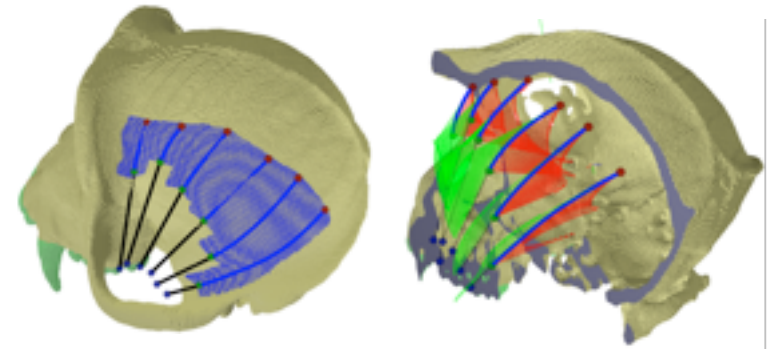Strong scaling
Horse head trabeculae
~200M elements
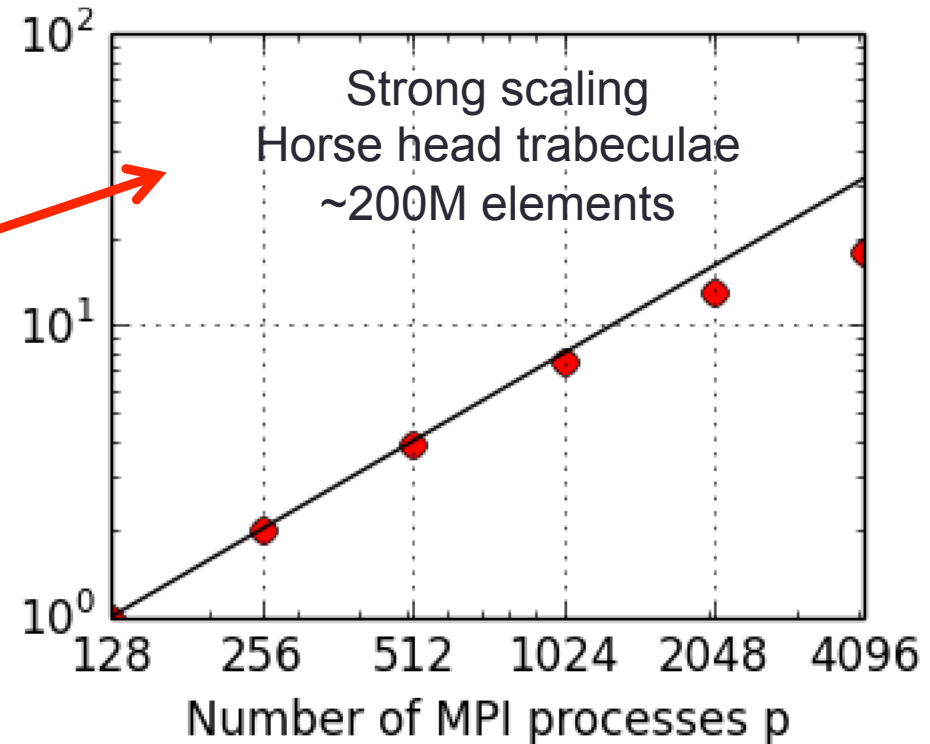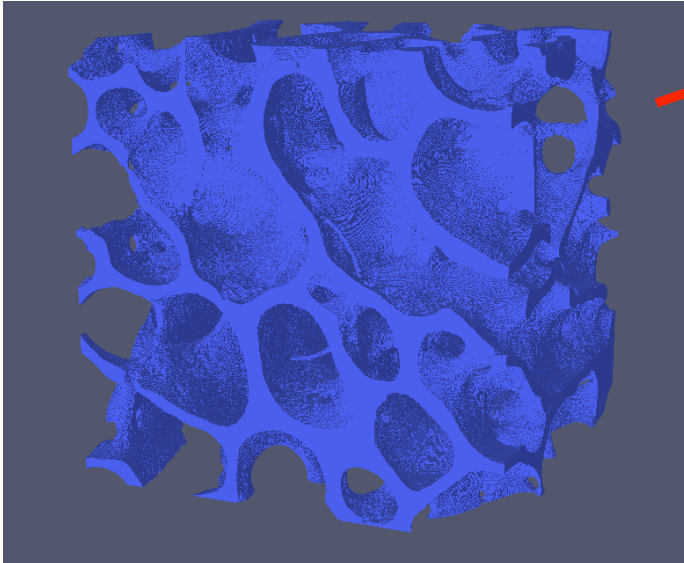
- Hundred of millions of elements, on thousands of cores, arbitrary number of materials
- Full open source release – ported to SourceForge
  - VOX-FE centrally available on ARCHER as an ARCHER module
  - Tutorials and user guide

eCSE : outcomes (cont.)

Remodelling
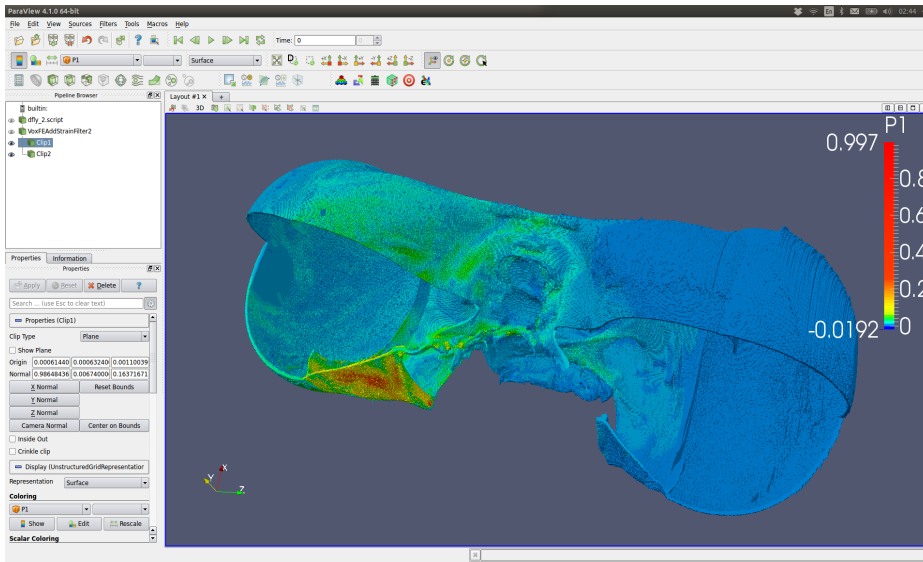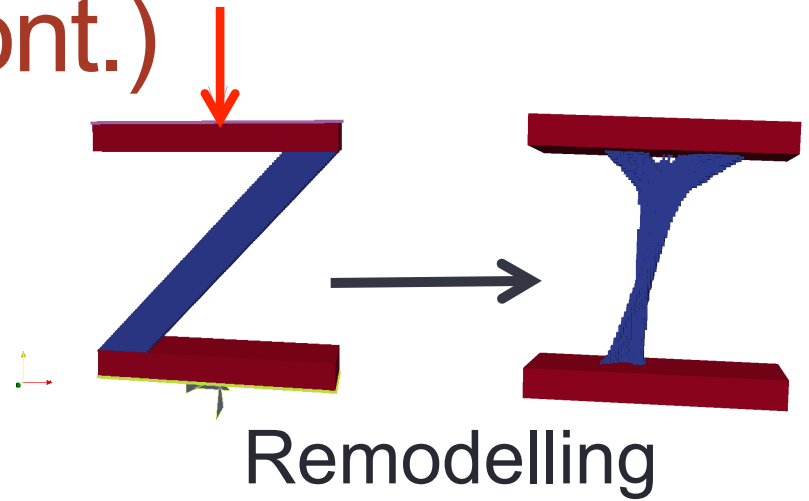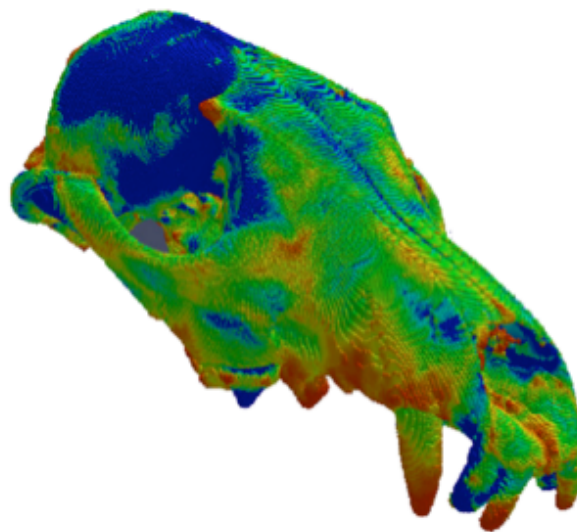
ParaView-based GUI

Muscle wrapping

eCSE : Outcomes (cont.)

- Overall financial saving/benefit ~10x for production jobs
- Produced final reports (including technical report)
- ARCHER white paper based on technical reports
    - http://archer.ac.uk/documentation/white-papers/
- ARCHER eCSE case study
- Webinar
    - https://www.youtube.com/watch?v=q7GD7Nv5LYs&feature=youtu.be

Summary

ARCHER eCSE programme provided opportunity for significant software development of VOX-FE, including new functionality that could potentially benefit a new user community.

http://www.archer.ac.uk/communicty/eCSE
support@archer.ac.uk