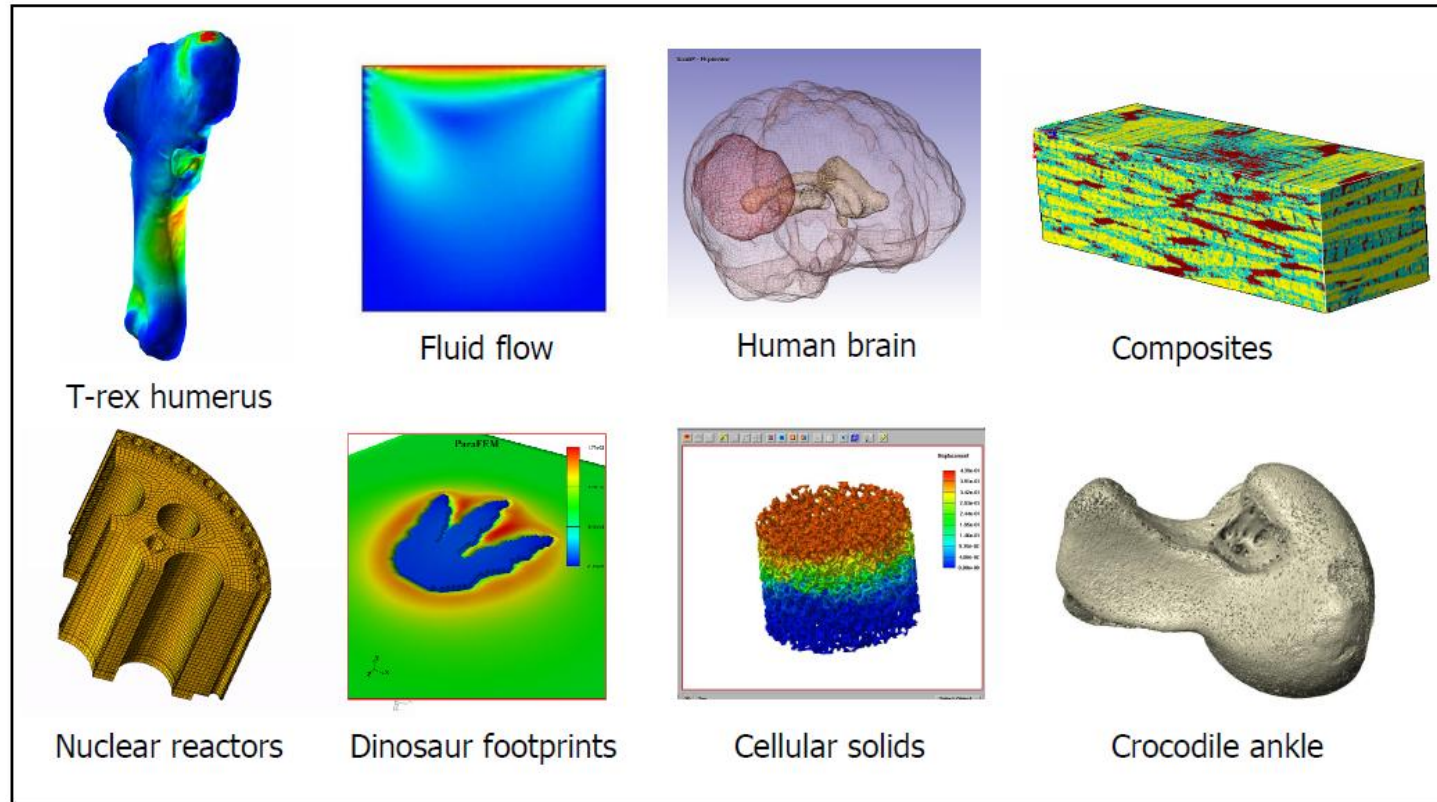


ParaFEM: Microstructurally Faithful Modelling of Materials



Louise M. Lever, University of Manchester
HECToR dCSE Seminar, NAG, Manchester, UK
9.30am Wednesday 5 October 2011

Overview

Background

1. The Speaker
2. ParaFEM
3. Manchester Imaging

Activities

1. dCSE Project
2. ParaFEM OSS Strategy

The Speaker

- Current employment, University of Manchester, 1993-present
 - Senior Consultant, IT Services for Research
 - Member of Eurographics UK Executive Committee

- Project manager and lead developer for AVS/Express development at Manchester
 - International AVS Centre
 - Multi-Pipe Edition
 - Parallel Edition

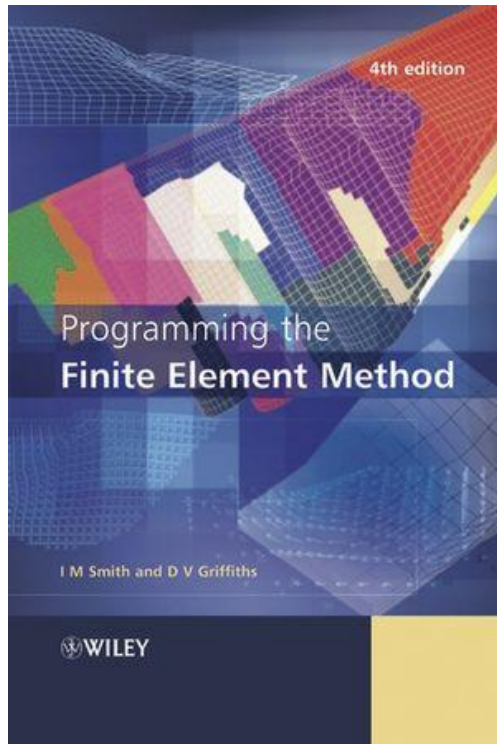
IT Services for Research @ UoM

- Supporting local researchers
 - Collaborative, research driven support model
- Supporting national services
 - CSAR (Manchester Computing)
 - National Grid Service
 - Access Grid
 - Data Management (JISC Madam project)
- Academic support via Manchester Informatics (Mi)
 - Key Themes
 - Computational Shared Facility

ParaFEM

- ParaFEM is a freely available, portable library of subroutines for parallel finite element analysis.
- The subroutines are written in FORTRAN90/95 and use MPI for message passing.
- It is an extension of the software developed in Smith I.M. and Griffiths D.V. "Programming the Finite Element Method", Wiley, 2004.
- The ParaFEM project owner is Dr Lee Margetts, an HPC specialist at the University of Manchester, UK. The latest release, version 2.0.819, was published on 29 July 2011.

Programming the Finite Element Method 2004



“Programming the Finite Element Method”

- I.M. Smith and D.V. Griffiths
- 4th Edition
- Easy to use example programs
- FORTRAN90/95
- Parallel versions

Over 500 Citations

Capabilities of ParaFEM

Static/Steady Analysis

- Static Linear Elastic Equilibrium (Small Strain)
- Static Elastoplastic Equilibrium
- Steady State Heat Flow & Seepage (Poisson equation)
- Steady Fluid Flow (Navier-Stokes equations)
- Large Strain Elasticity (St Venant-Kirchoff Material)

Transient Analysis

- Explicit/Implicit Transient Flow
- Coupled Transient Deformation/Flow
- Dynamic Equilibrium of Elastic/Elastoplastic Solids

Others

- Eigenvalues/vectors (elastic solids)

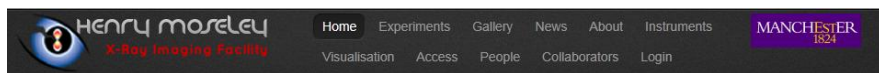
Manchester Imaging

Manchester X-Ray Imaging Facility

- New facility at the University of Manchester
- Includes existing Henry Moseley X-Ray Imaging Facility (HMXIF) in Manchester
 - <http://xray-imaging.org.uk/>
- And the University of Manchester has a beamline at the Diamond Light Source Facility
- New MXIF Experiment Management System
 - <http://www.manchester.ac.uk/imaging> [Future]

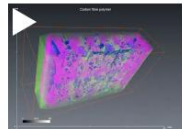
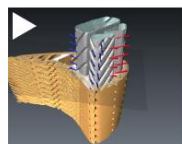
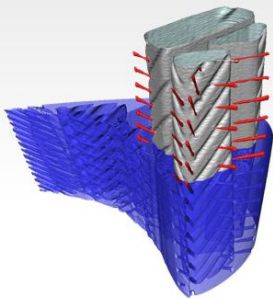


Experiment Management System



3D X-ray vision is no longer solely the subject of movies and comic books.

Today's researchers from cutting edge fields such as aeronautical, materials and biological tissue engineering are gaining new insights by using 3D X-ray Computed Tomography (CT).

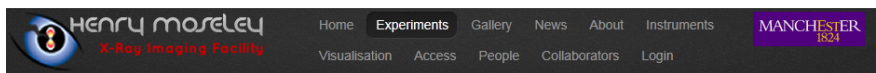
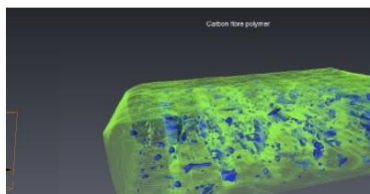


What is 3D X-ray Computed Tomography?

So what is 3D X-ray Computed Tomography (CT) and how does it work? Well, it works along the same lines as when a doctor takes an X-ray of a broken bone. However, rather than taking just one 2D X-ray picture, known as a radiograph, hundreds or even thousands of radiographs are taken of the object as it is rotated through 360°. The series of 2D radiographs are then reconstructed into a 3D image using sophisticated software packages coupled with powerful computers. The real advantage of CT lies in the fact that a virtual replica is created where one can slice through the layers of the object to reveal its internal structure, akin to peeling an onion. Further, in some cases one can then follow its structure as it changes over time.

Originally CT was developed in the 1970's for medical imaging and today it is routinely used in both state and private medical centres for diagnosis purposes, such as for the detection of tumours, etc. Recently, CT has seen an increased use in preventative medicine by the use of body scans as part of a general health check.

Although CT has been around for the last 40 years, it is still the best 3D imaging technique available.



Proposals

Characterization of process parameters of Mg composites produced by hot pressing.

Written by: [Hanna Marta Myalska](#)
Wednesday, 20 July 2011 13:47

Last Updated on Wednesday, 14 September 2011 13:57

Short Description: Material was obtained from magnesium and silicon dioxide powders mixtures by hot pressing. Three different volume fractions of silicon dioxide were applied in initial powders mixtures used for sintering. An effect of reaction between components will be characterized with X-ray tomography.

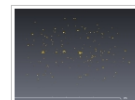
Scanner: Xradia MicroXCT

Material Type: Metals

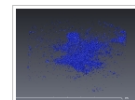
Other Material: Composites

Features of Interest: Mg2Si, porosity

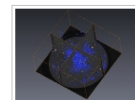
Experiment Gallery:



Mg sample with 10% SiO₂_3



Mg sample with 10% SiO₂_2



Mg sample with 10% SiO₂_1



Mg sample with 6% SiO₂_3

Related Content: [List of Scan Records, Articles and Publications](#)

Determination of the Re-passivation Kinetics of Pits in Pure Aluminium

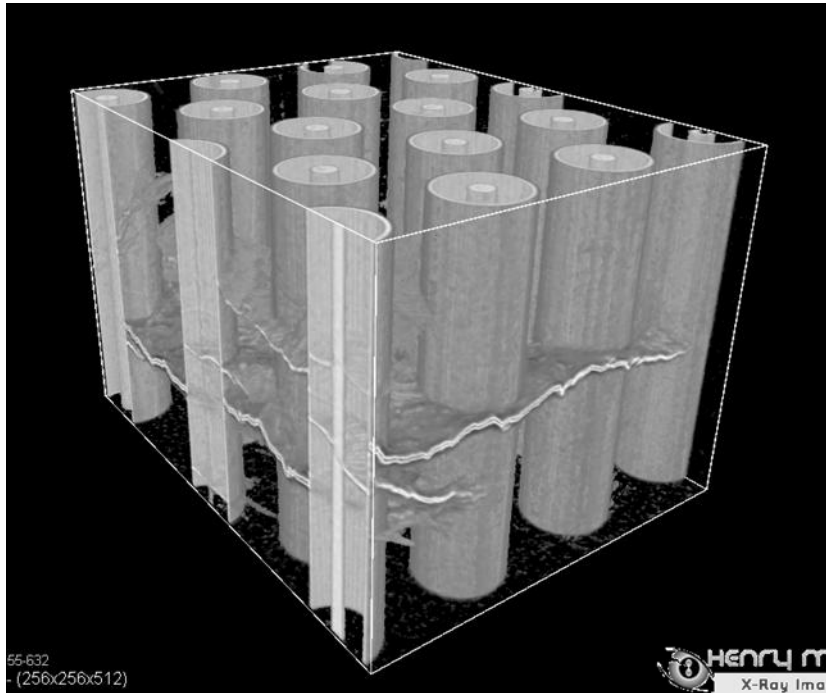
Written by: [Dirk Lars Engelberg](#)

Tuesday, 19 July 2011 15:41

Last Updated on Monday, 22 August 2011 10:33

Short Description: Corrosion pit growth studies will be carried out, in-situ, in a small electrochemical cell using artificial pencil electrodes with aluminium wires of 15, 50 and 125 µm diameter. The experiments will be conducted in dilute HCl solution (1 M) under external potential control. It is proposed to monitor changes in the morphology of various diameter artificial pits (15, 50 and 125 µm diameter wire), in-situ, using radiography over a range of applied

HMXIF Examples



Incremental crack growth in
titanium/silicon carbide



Pacemaker battery



Imaging

- Engineers historically used imaging techniques to simply “look at” materials
- Now using imaging to create the models
- And model how they behave
- HPC requirements at most stages of their workflow

Webbed Tracks From Non-webbed feet

Dr Phil Manning and Dr Peter Falkingham

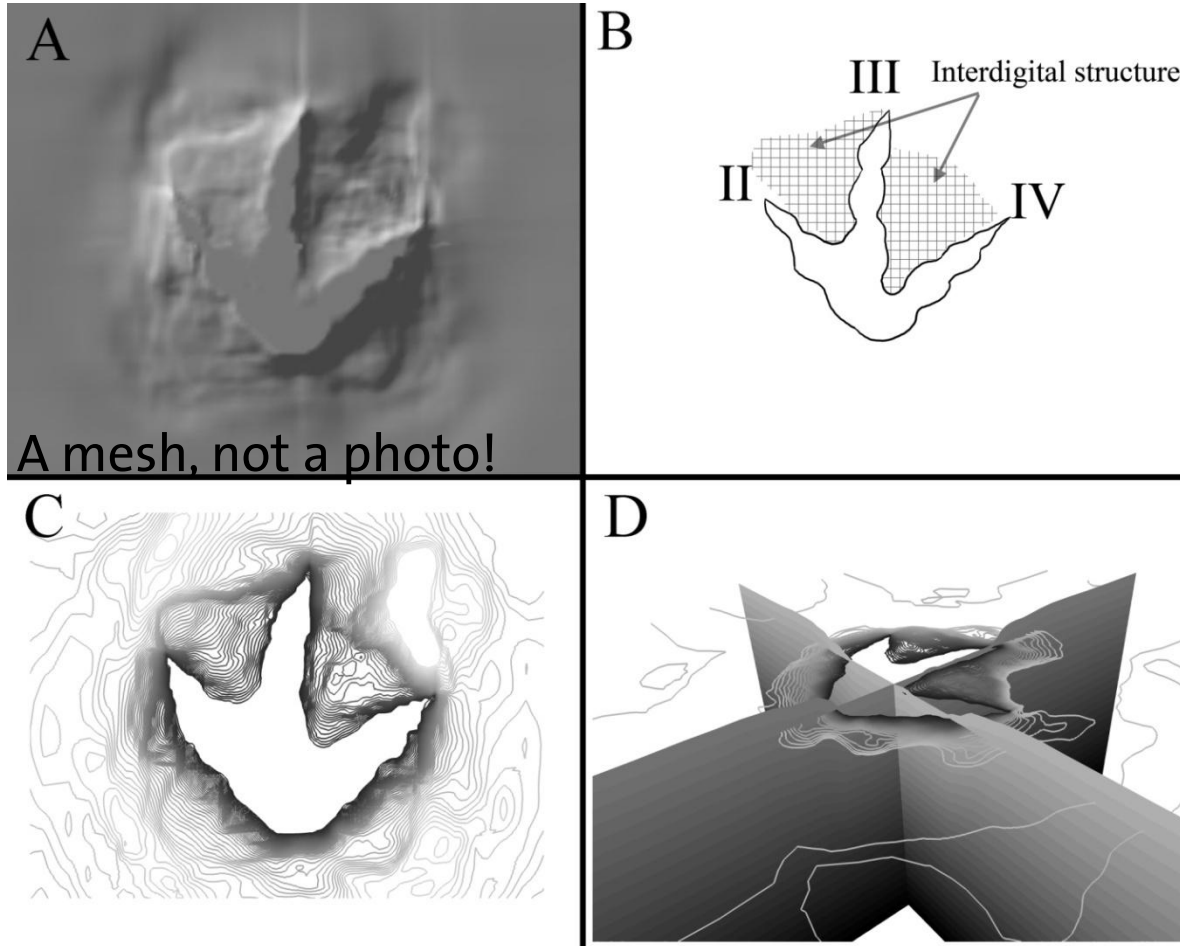


Image Based Meshing

Dr Paul Mummery and Dr Philippe Young

- Tomography follows a “Moore’s Law” for image resolution and number of detectors. 2000^3 to 4000^3 voxels etc
- Requires “Out-of-core” and parallel grid based meshing
- Meshes with 2+ billion element models created

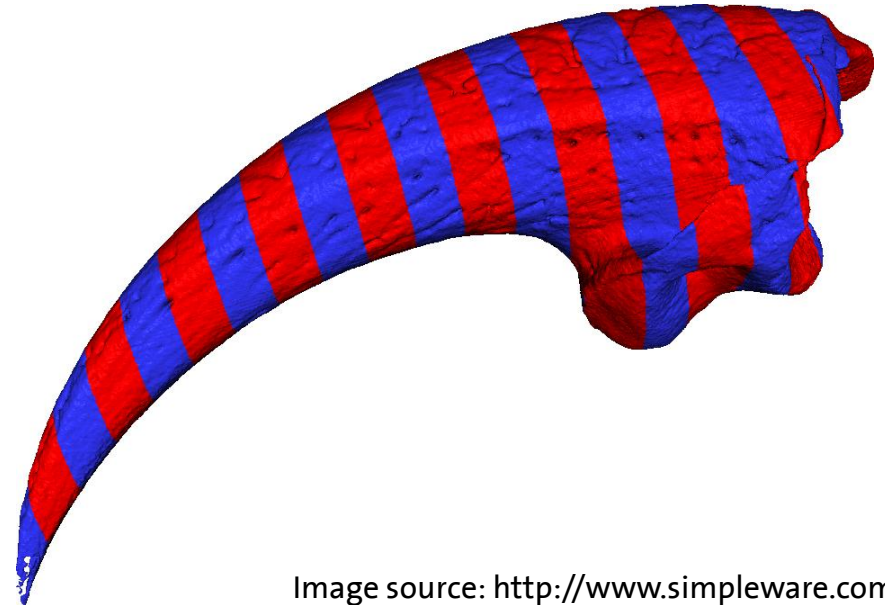


Image source: <http://www.simpleware.com>

Multiscale Modelling

Dr Phil Manning and Dr Bill Sellers

- FE based micro-scale to macro-scale homogenization
- KUBC, SUBC and periodic boundary conditions
- Unit cell or RVE based characterization
- Based on separation of length scales

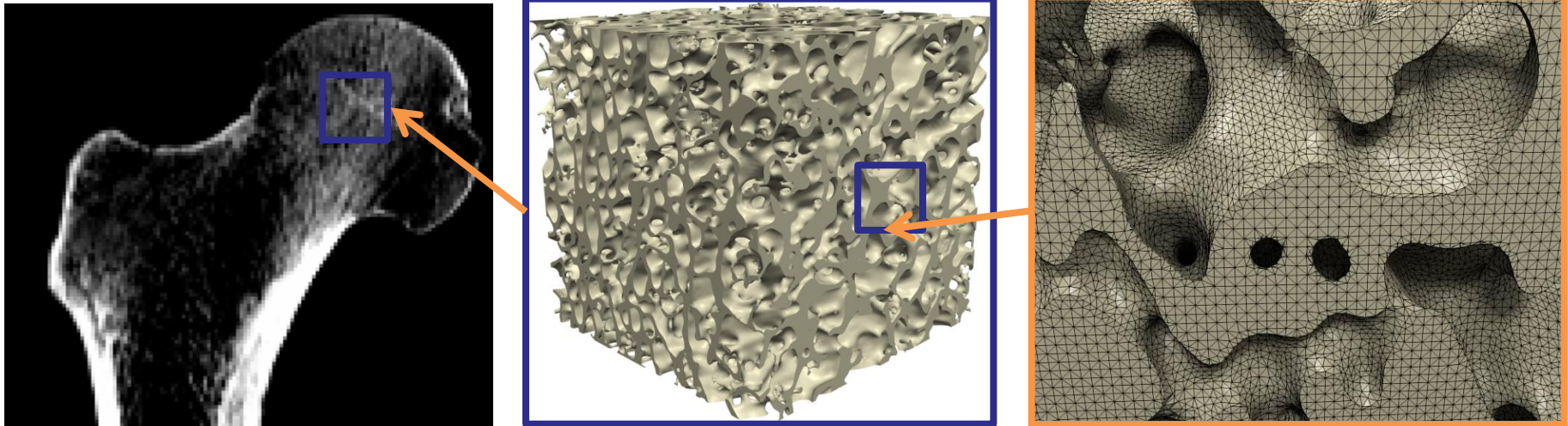


Image source: <http://www.simpleware.com>

Multiscale Modelling

- KUBC Kinematic Uniform Boundary Conditions - Apply the macro strain to the micro-scale, solve for micro stresses and compute macro stress. Macro stress-strain relationship gives "effective" Young's modulus.

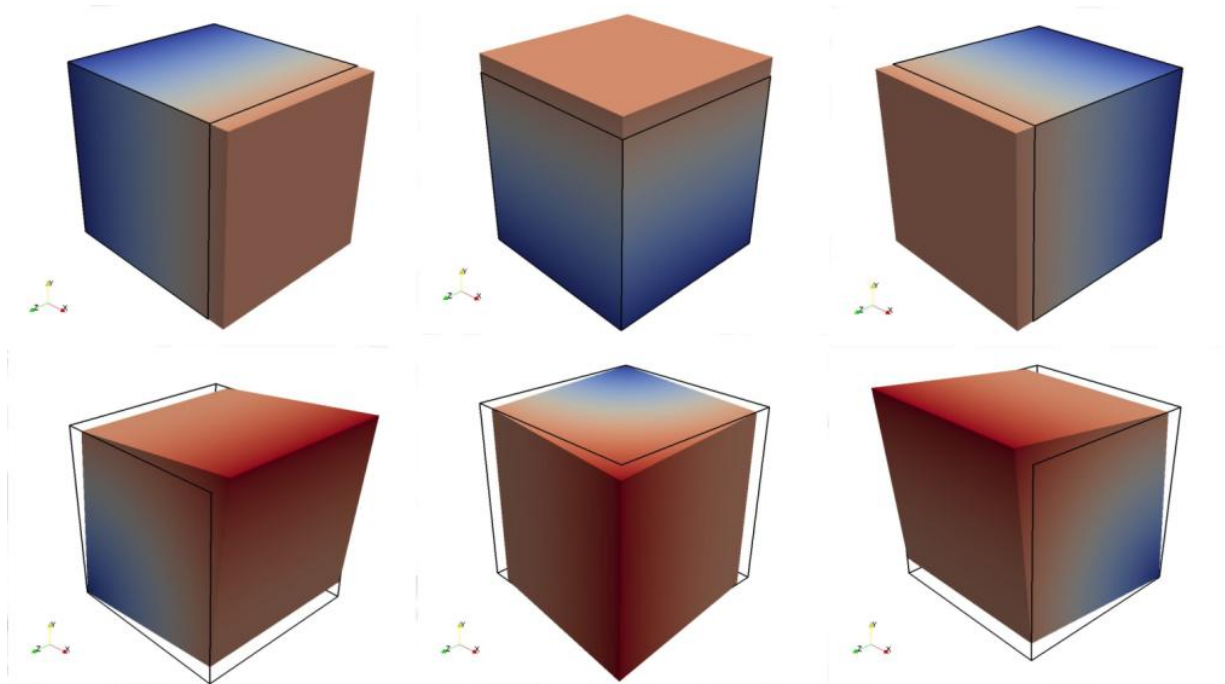
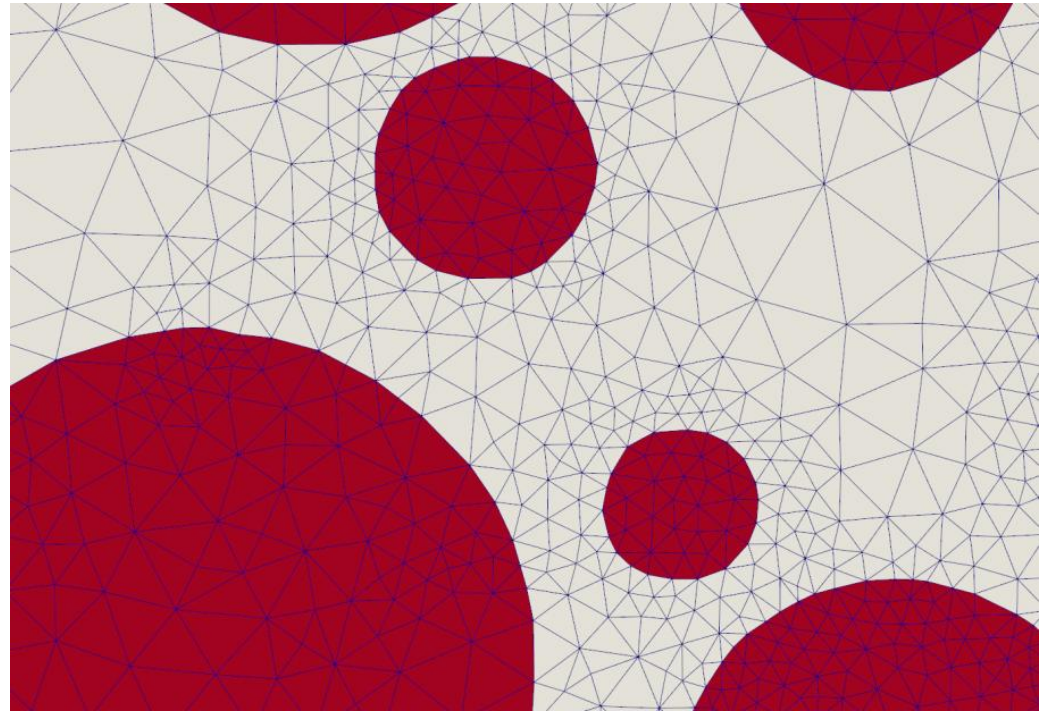
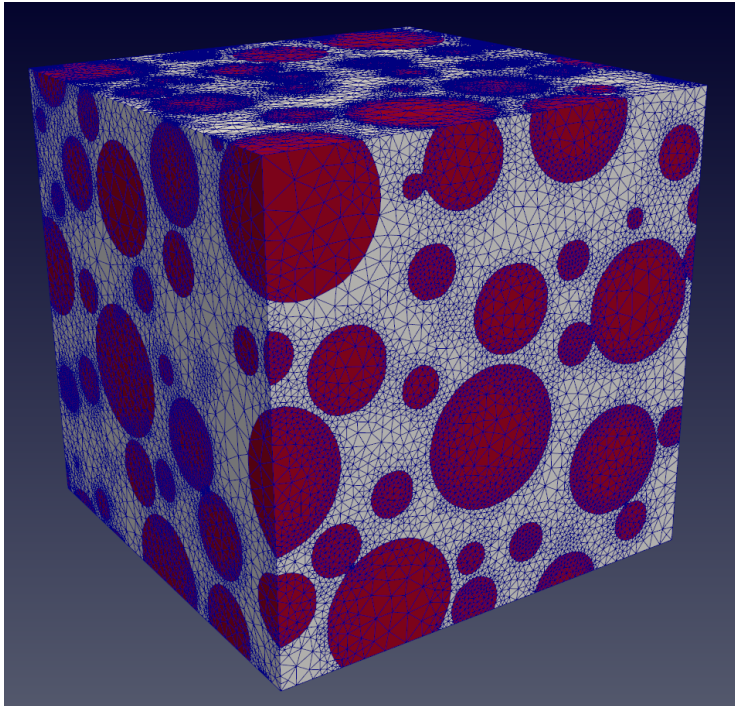


Image source: Peter Falkingham

Multiscale Modelling

Dr Paul Mummery and Dr Philippe Young

- EDF homogenization benchmark problem
- 330+ million elements



HECToR GPU Testbed

Dr Paul Mummery and Dr Michael Bane

- Pilot evaluation of GPU acceleration for iterative solvers
- ParaFEM can be easily adapted to run on multiple compute nodes with GPU accelerators
- GPU implementation of the iterative solver needs to accelerate large loops of small matrix-vector multiplies

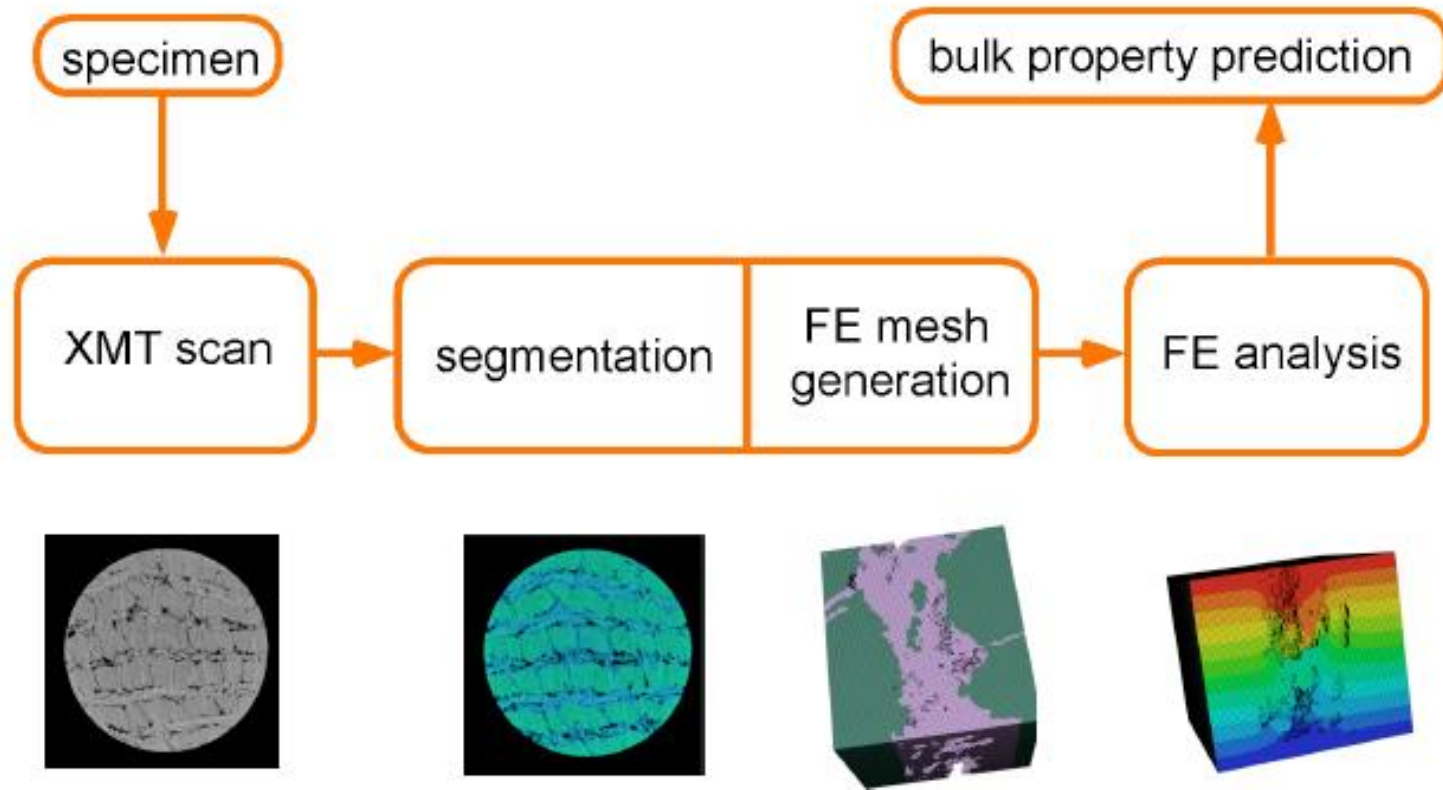


- Some special cases, voxelated meshes from CT images very suitable
- Single matrix, multiple vectors – high level memory reuse

dCSE Project

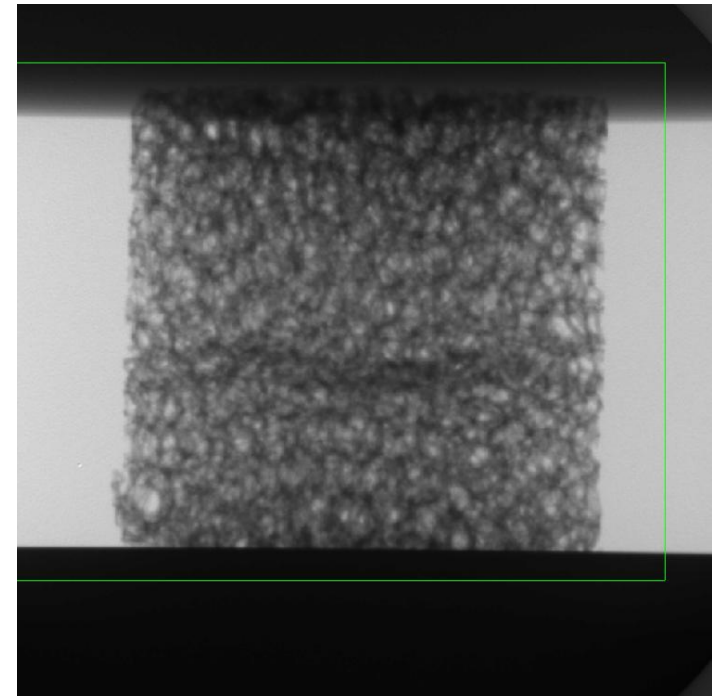
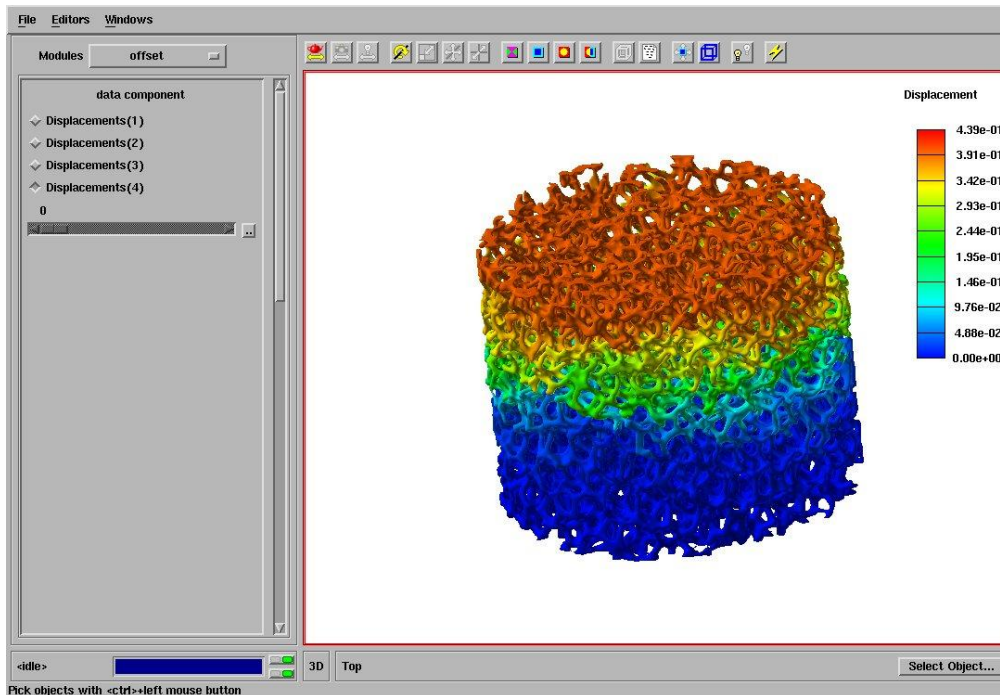
Image Based Modelling

Professor Philip Withers & Professor Paul Mummery



Supporting Henry Moseley X-Ray Imaging Facility
<http://xray-imaging.org.uk/>

- ParaFEM interface to Abaqus UMATs (User Material Subroutines)
- Visualization of large datasets: ParaFEM-Viewer (MRBV), ParaView
- Example below 170M element model of aluminium foam



Purpose of dCSE

- The goal is to make it easier to use ParaFEM
- By allowing addition of new material models
- And enabling the visualization of large models
- Commercial sponsors have people wanting to use ParaFEM
 - EDF; Microsoft; ESA; Rolls-Royce; and SMEs (using PaaS)
- Would like them to move away from systems like Abaqus
 - Problem size limitations
- While simultaneously not wanting them to abandon Abaqus
 - It's a closed environment and provides most things

- User *MA*terial Types are Fortran subroutines that implement a specific material behaviour
- Can add to Abaqus to extend modelling options
- Provide mechanism for users to quickly add the same UMATs to ParaFEM
- Not straightforward because the implementation depends on problem type and there are a huge number of types of problem

Why use UMATs

- Different types of material behaviour require different types of solutions
- ParaFEM is limited in number of models supported
- For Large Strain Deformation a new type of model was required
- Materials like brain, skin and other tissue do not behave like traditional engineering materials
- Maths for aluminium block (small strain) is not the same as bio-material (large strain)

UMAT Fortran API

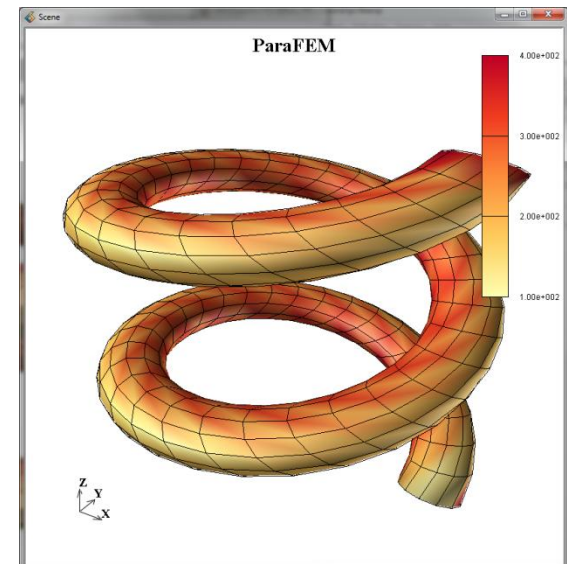
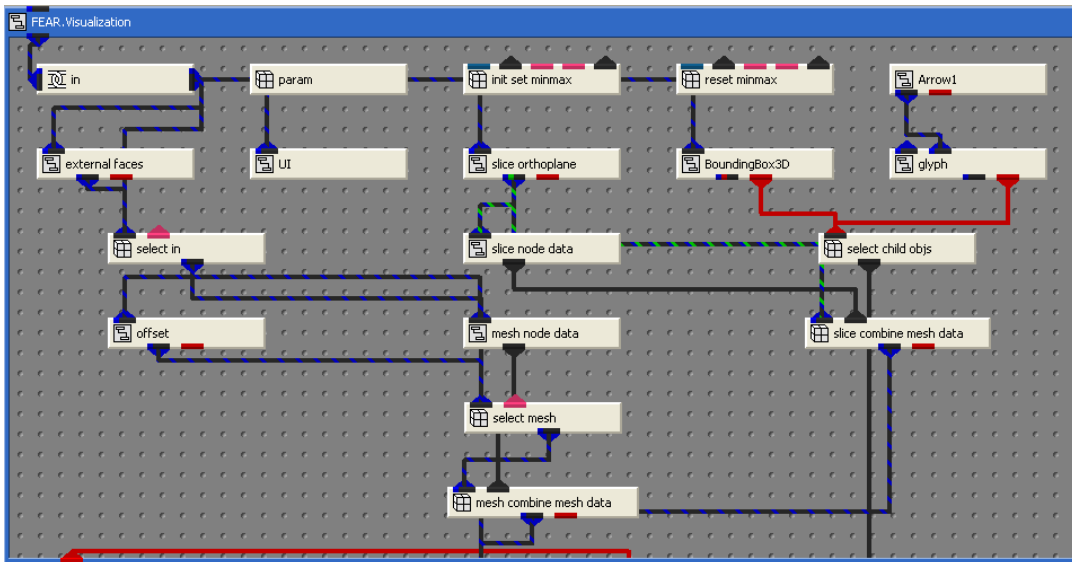
```

xx1.f90 - paraferm - A Portable Librar...
192
193 ! -----
194 ! 8. Element stiffness integration and storage
195 !
196 !     Note that the DEEMAT and UMAT subroutines are currently outside the loop
197 !     elements_3. This is only correct when all the elements are of the same
198 !     type and have the same material properties.
199 ! -----
200
201     CALL sample(element,points,weights)
202
203     !   dee = zero
204     !   CALL deemat(e,v,dee)
205
206
207     dee = zero
208     CALL umat(sigma,statev,dee,sse,spd,scd,rpl,ddsddt,drplde,drpldt,stran,    &
209              eps,time,dtime,temp,dtemp,predef,dpred,cmname,ndi,nshr,    &
210              nst,nstatv,props,nprops,points,drot,pnewdt,celent,dfgrd0,dfgrd1, &
211              iel,npt,layer,kspt,kstep,kinc)
212
213     storkm_pp      = zero
214
215     elements_3: DO iel=1,nels_pp
216         gauss_pts_1: DO i=1,nip
217             CALL shape_der(der,points,i)
218             jac  = MATMUL(der,g_coord_pp(:, :, iel))
219             det  = determinant(jac)
220             CALL invert(jac)

```

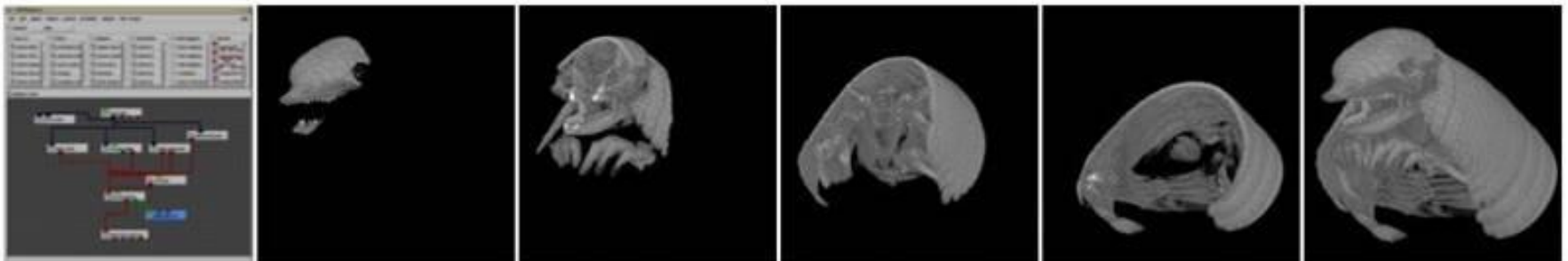
ParaFEM-Viewer

- Model viewer built on AVS/Express
- Custom reader for ParaFEM file format
- Custom application to enable users to visualize data rather than building visualization networks



- Massive Remote Batch Visualizer
- Extension of AVS/Express Parallel Edition
 - Using Multi-Pipe and Distributed Data Renderer (DDR)
 - And Parallel Support Toolkit (PST) for computation
 - Parallel rendering without need for graphics hardware
 - Ported to HECToR by George Leaver in dCSE project

- Some problems with MPI on HECToR to overcome
 - DDR already fully MPI based but no MPI on HECToR head node
- Focuses primarily on rendering of structured volumes
 - Includes MPI and thread-based direct volume renderer

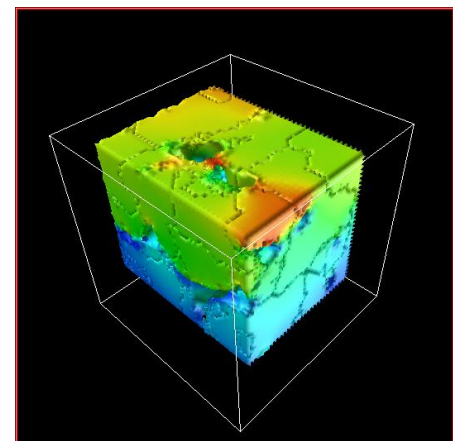
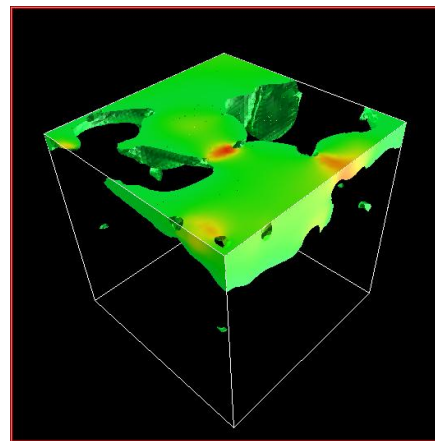
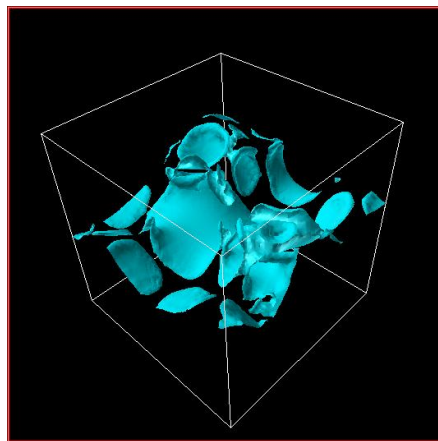
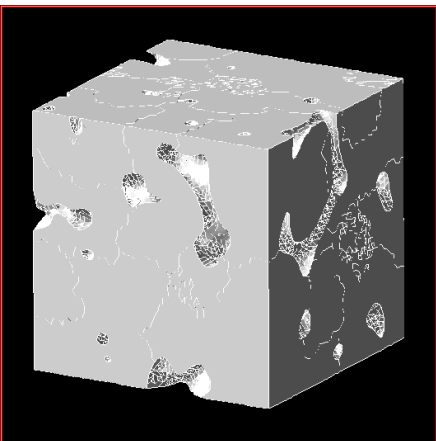


Porting ParaFEM-Viewer to MRBV

- Wanted to port ParaFEM-Viewer
 - Write parallel IO for ParaFEM file format
 - Or convert to existing supported format such AVS UCD
 - Replace serial modules in application with their parallel counterparts
 - Add animation scripts to enable batch usage

Experience with MRBV

- Developed conversion scripts to single and multi-file UCD
- Can read data in
 - Serial: is then decomposed and distributed by parallel toolkit
 - Parallel: each node reads a pre-decomposed file
- And see the model and results



Problems with MRBV

- Problems encountered included
 - Limitations of multi-file UCD: no time steps
 - Limitations of parallel toolkit: no element data
- Effort to create a native parallel reader would have to include further development of AVS/MRBV
 - Beyond scope of this dCSE project
- Licensing
 - Manchester is only academic site with license
 - Very likely to change in 2012
 - Similar issue for desktop users
 - And concern for ParaFEM open source plans

Using ParaView

■ Benefits

- Open Source, freely customizable, multi-platform
- Built on comprehensive and sophisticated VTK library
- Many visualization and parallelization strategies

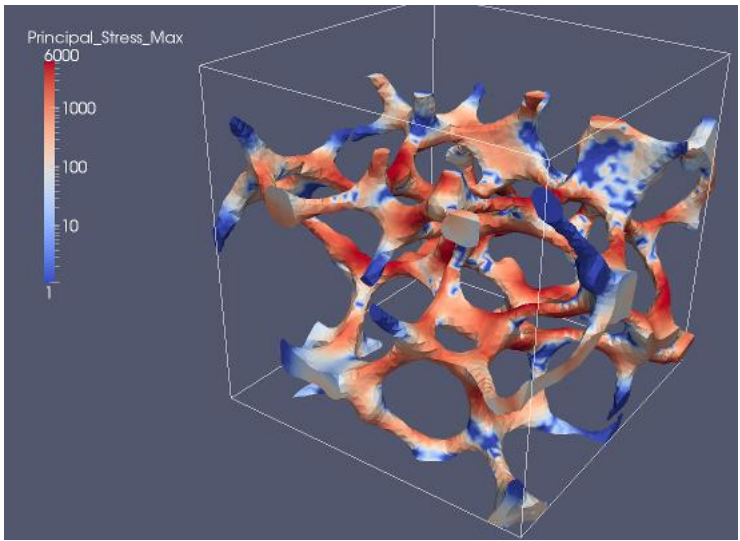
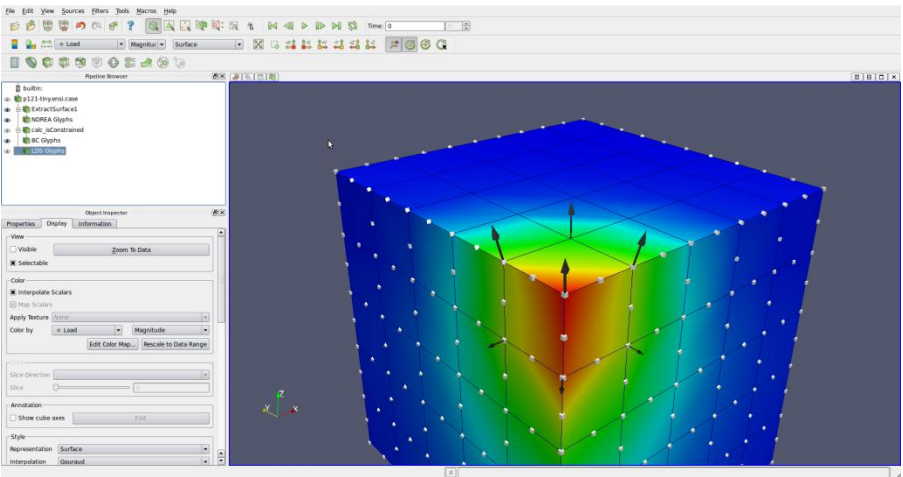
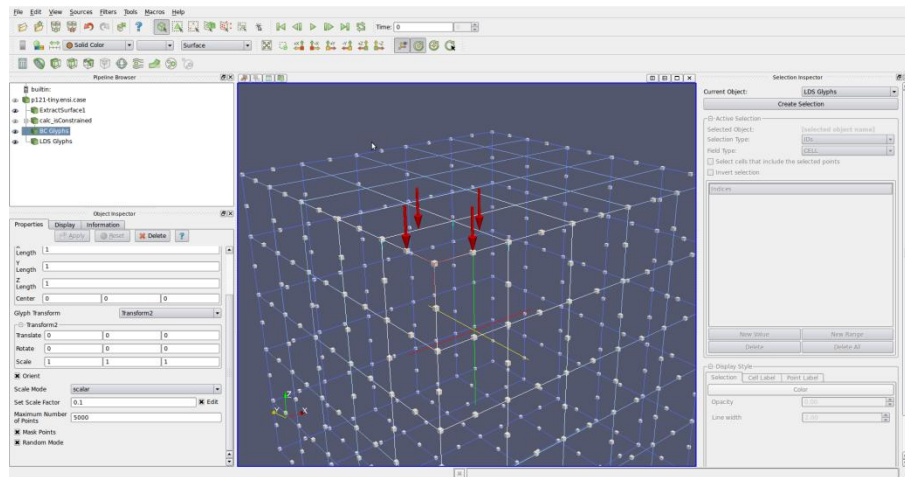
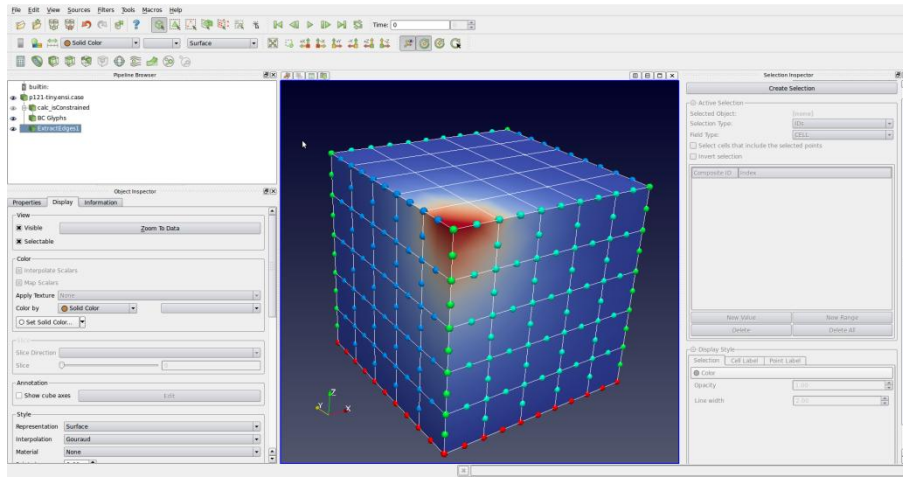
■ Drawbacks

- Takes users (initially) back to hands-on control of visualization pipeline
- Greater effort to provide a custom interface

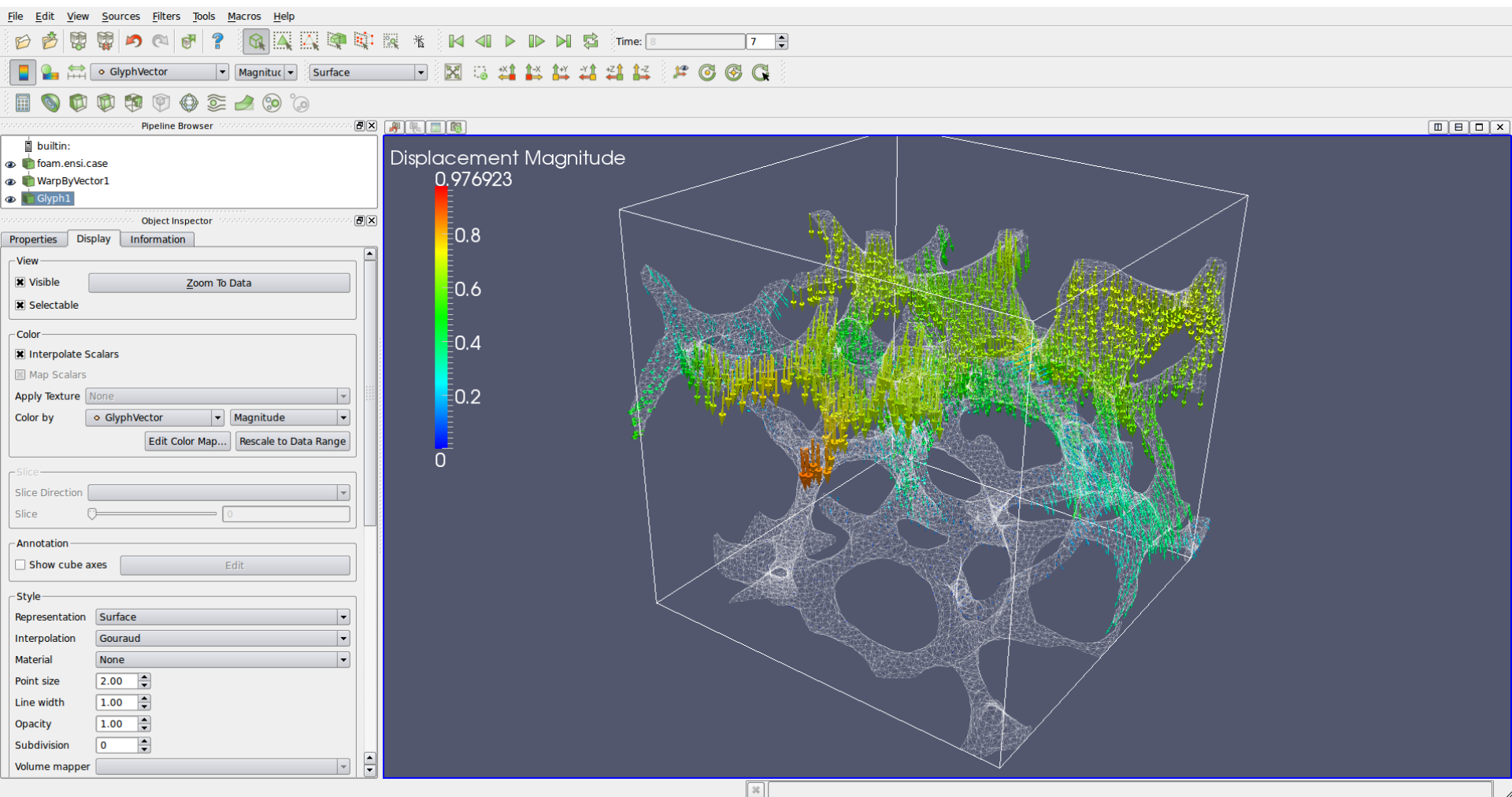
Moving to ParaView

- Data format handling
 - No native ParaFEM reader for ParaView
 - Beyond scope of dCSE project
 - Opted for conversion to supported EnSight Gold Format
- Issues
 - ASCII only at the moment
 - VTK reader code has errors and does not load partial data
 - VTK code fixed but not submitted yet
 - File access every time on loading of each time step
 - Seems slow in comparison to AVS/Express

ParaFEM Results in ParaView



ParaFEM Results in ParaView



Remaining Work on dCSE

- Tidying up of software
- Looking for more UMATs
- Load-balancing tests
 - ParaFEM is perfectly balanced for simple material types
 - Have non-linear parts in certain regions
 - Will measure and profile how non-linearity affects load-balancing
- Have already integrated METIS tools into ParaFEM suite
 - Re-partition with METIS
 - See if we get better load-balancing with METIS partitions
 - Have two strategies to compare

6. ParaFEM OSS Strategy

Google Code Platform for Developers

File Edit View History Bookmarks Tools Help

http://code.google.com/p/paraferm/

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A Portable Library for Parallel Finite Element Analysis

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Project Information

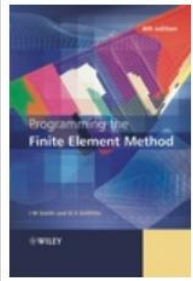
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Code license
[New BSD License](#)

Labels
 FEM, BEM, Mechanics, HPC, MPI, Fortran, Grid, Analysis, CAE, PDE, Engineering, FiniteElement, Windows, Linux

Members
[drleemargetts](#), [louise.m.lever](#)
 3 committers

Welcome to the ParaFEM Project



ParaFEM is a freely available, portable library of subroutines for parallel finite element analysis. The subroutines are written in FORTRAN90/95 and use MPI for message passing. It is an extension of the software developed in Smith I.M. and Griffiths D.V. "Programming the Finite Element Method", Wiley, 2004. The ParaFEM project owner is Dr Lee Margetts, an HPC specialist at the University of Manchester, UK. The latest release, [version 2.0.819](#), was published on 29 July 2011. [Download here](#).

+1 1

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Google Code Platform

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http://code.google.com/p/parafem/source/browse/trunk/parafem/src/programs/4th_ed/p121/p121.f90


☆ parafem

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A Portable Library for Parallel Finite Element Analysis

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Source path: [svn/](#) [trunk/](#) [parafem/](#) [src/](#) [programs/](#) [4th_ed/](#) [p121/](#) p121.f90 [< r571](#) [r857](#)

1 PROGRAM p121
2 !
3 ! Program 12.1 three dimensional analysis of an elastic solid
4 ! load control or displacement control
5 !
6
7 USE precision ; USE global_variables ; USE mp_interface
8 USE input ; USE output ; USE loading
9 USE timing ; USE maths ; USE gather_scatter
10 USE partition ; USE elements ; USE steering ; USE pcg
11
12 IMPLICIT NONE
13
14 !-----
15 ! 1. Declare variables used in the main program
16 !-----
17
18 ! neq,ntot are now global variables - not declared
19

Change log
[r579](#) by lee.margetts@manchester.ac.uk on Jun 7, 2011
[Diff](#)
PRINT* statements removed from p121.f90

Go to:
Double click a line to add a comment

Older revisions
[r571](#) by lee.margetts@manchester.ac.uk on Jun 6, 2011
[Diff](#)

HECToR dCSE Seminar, NAG, Manchester, 9.30am Wednesday 5th October 2011 43

<http://parafem.org.uk>

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ParaFEM

The freely available portable library
for parallel finite element analysis.

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Thursday, September 01,
2011

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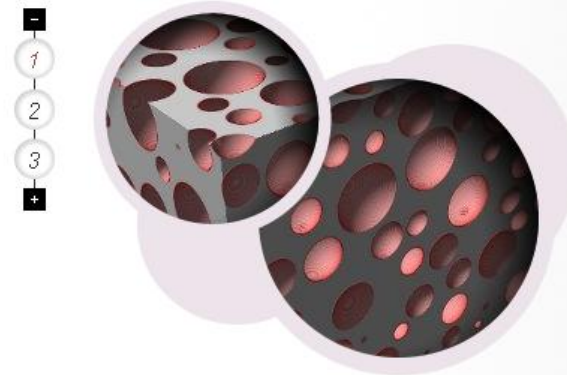
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benchmarking of materials modelling

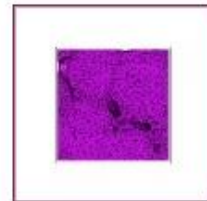
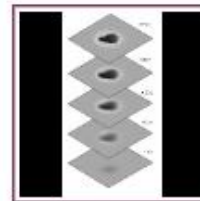
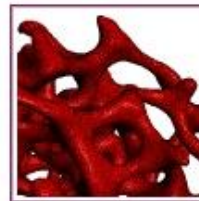
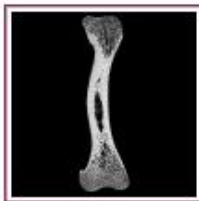
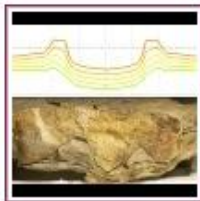
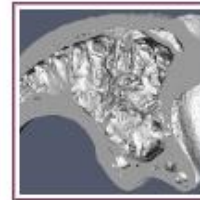
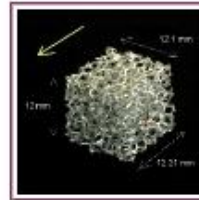
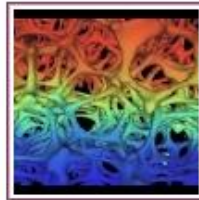
Engineers at EDF are developing a Materials
Modelling Platform that will incorporate a number of
open source software programs and provide
interfaces for commercial applications.

[+ read the full story](#)



Joomla Community Building Platform

Images from the Gallery



Latest Projects

- Programming the Finite Element Method
- Goldilocks and Dinosaur tracks
- Benchmarking for EDF's Materials Modelling Platform

Latest News

- Call for Papers: ECT2012
- Seventh International PhD & DLA Symposium
- VACANCY - Modelling of Phase-Separation in Heterometallic Nanoparticles

Latest Comments

- Michael, great! I think we wont make the deadline ...
- Lee, I'm up for this. I've a few ideas of using va...
- The following extract from the article is of parti....

Tag Cloud

ARPACK **Cloud Computing**
Composites Engineering
 Exascale Fossil Tracks **GPU**
 HLRS **HPC** Job METIS
 Multicore **NAFEMS**
 Nanotechnology Optimization

Joomla back end for paraferm.org.uk

Joomla! ParaFEM Version 1.5.23

Site Menus Content **Components** Extensions Tools Help CCK

Preview 0 1 Logout

New Article

Menus

User Management

Global Configuration

AllVideos Reloaded

Banner

Check in/out

Community Builder

Contacts

CQL Custom Quick Icons

JCE Administration

JComments

jDownloads

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jSeblod CCK

News Feeds

Phoca PDF

Polls

RokBridge

RokCandy

Search

uddelM

Web Links

Frontpage

Categories

Users

Configuration

Category Manager

Image Manager

Comments Manager

Image Upload

Batch Upload

FTP Upload

Java Upload

Configuration Manager

CSS Manager

Migration Manager

Maintenance Manager

Plugins

Logged in Users

#	Name	Group	Client	Last Activity	Logout
1	zzalsm3	Super Administrator	administrator	0.0 hours ago	

Articles with Duplicate Meta Descriptions

Articles with Duplicate Title Aliases

Articles with Duplicate Titles

JComments Latest Backend

Recent added Articles

Menu Stats

Popular

How well are we doing?

Google Analytics

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Dashboard

Intelligence Beta

Visitors

Traffic Sources

Content

Goals

Customised Reporting

My Customisations

Custom Reports

Advanced Segments

Intelligence Beta

Email

Help Resources

About this Report

Conversion University

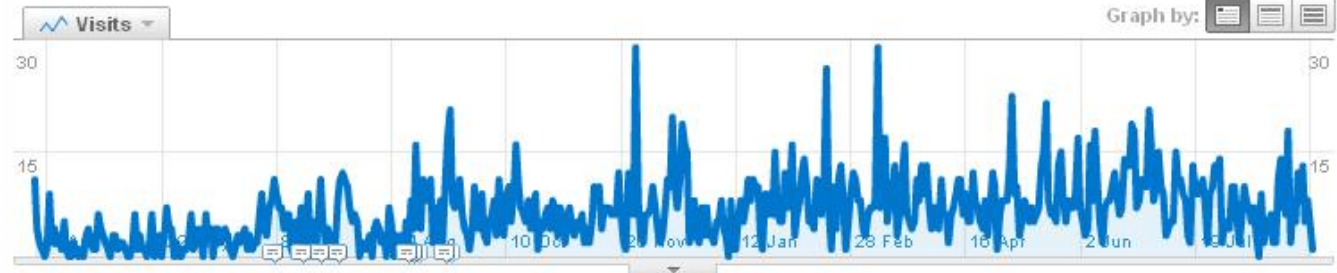
Common Questions

Export Email





Advanced Segments: All Visits

Dashboard

31 Mar 2010 - 5 Sep 2011



Site Usage

 3,358 Visits 33.17% Bounce Rate 19,336 Pageviews 00:05:34 Avg. Time on Site 5.76 Pages/Visit 36.03% % New Visits

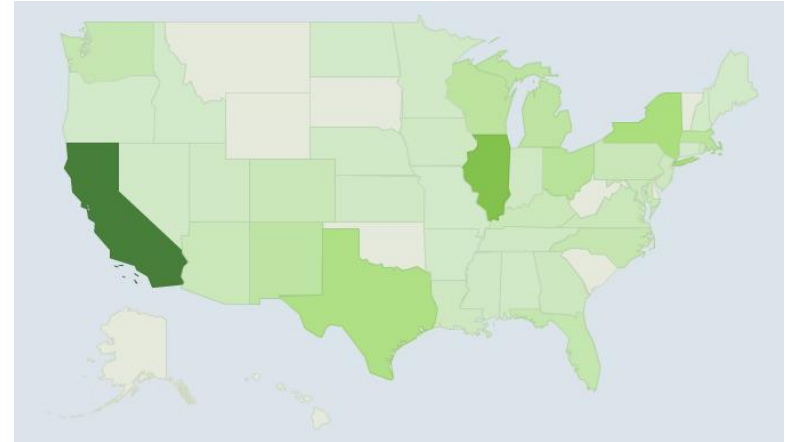
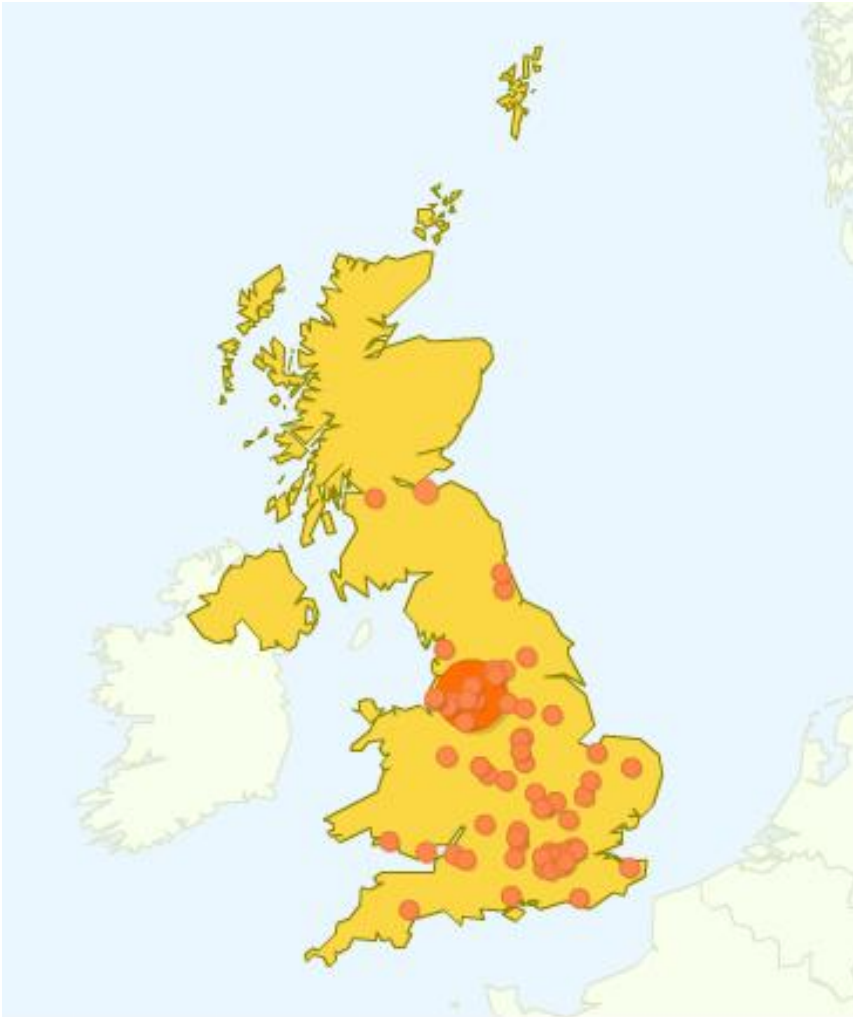
Visitors Overview

Map Overlay

Visitors - code.google.com/p/paraferm



Visitors - code.google.com/p/paraferm



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For further details, please contact

louise.lever@manchester.ac.uk

lee.margetts@manchester.ac.uk

<http://www.rcs.manchester.ac.uk/aboutus/staff/LouiseLever>