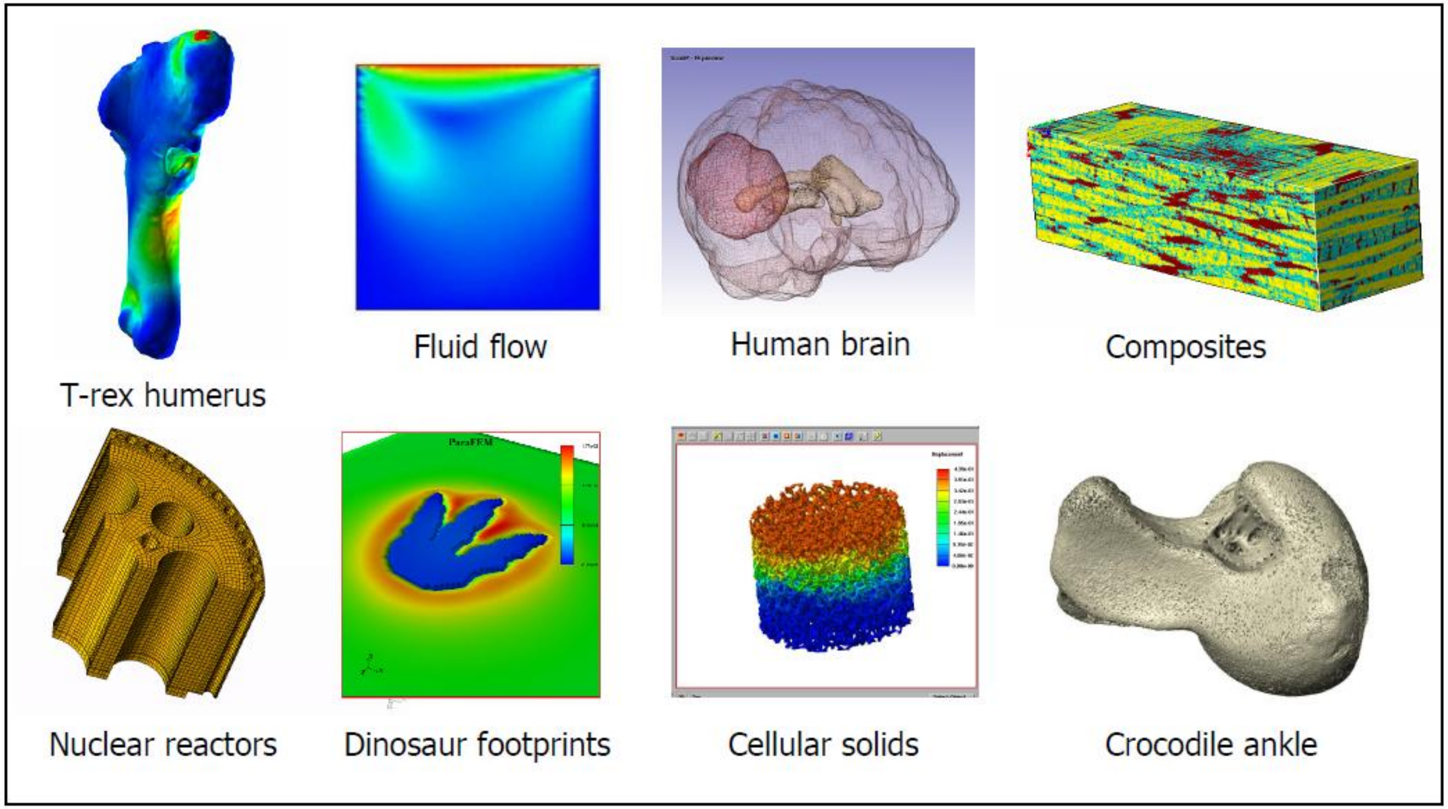
# ParaFEM: Microstructurally Faithful Modelling of Materials




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

# Biography

- 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

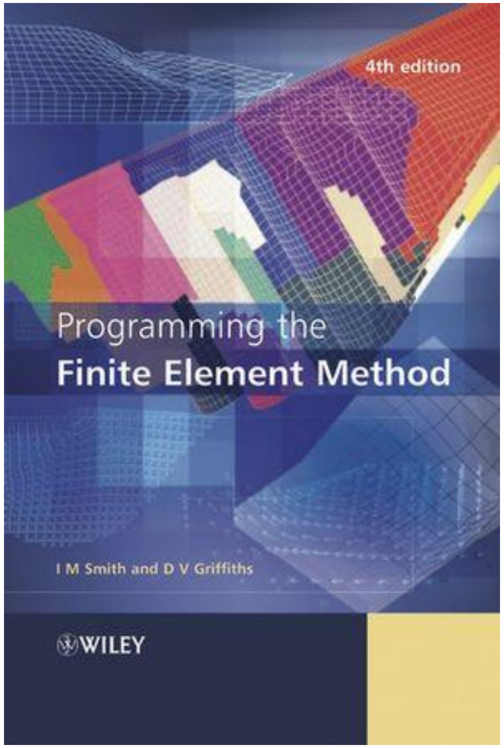
- Supporting local researchers
  - Collaborative, research driven support model
- Supporting national services
  - CSAR  (Manchester Computing)
  - National Grid Service
  - Access Grid
  - Data Management (JISC Madam project)
- Academic support via Manchester Informatics (Mi)
  - Key Themes
  - Computational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

# ParaFEM

# ParaFEM

- 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)

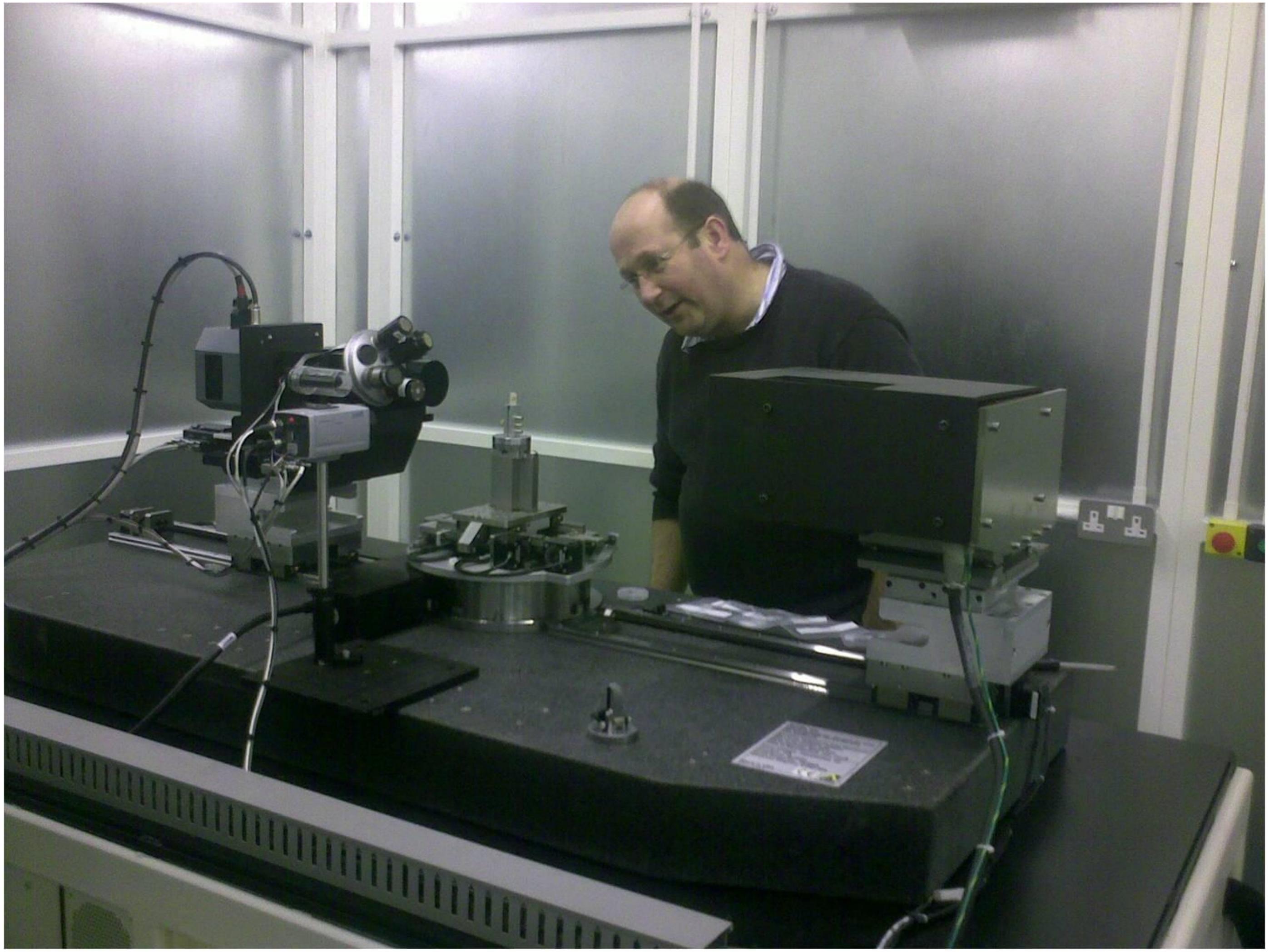
# Manchester Imaging

# 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]

# HMXIF



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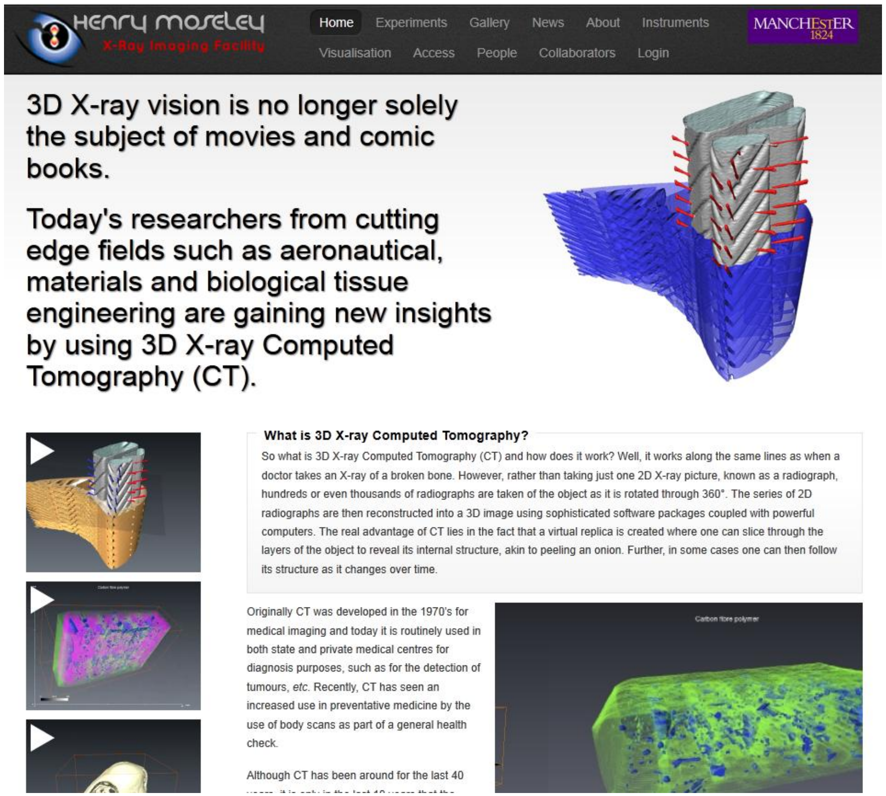
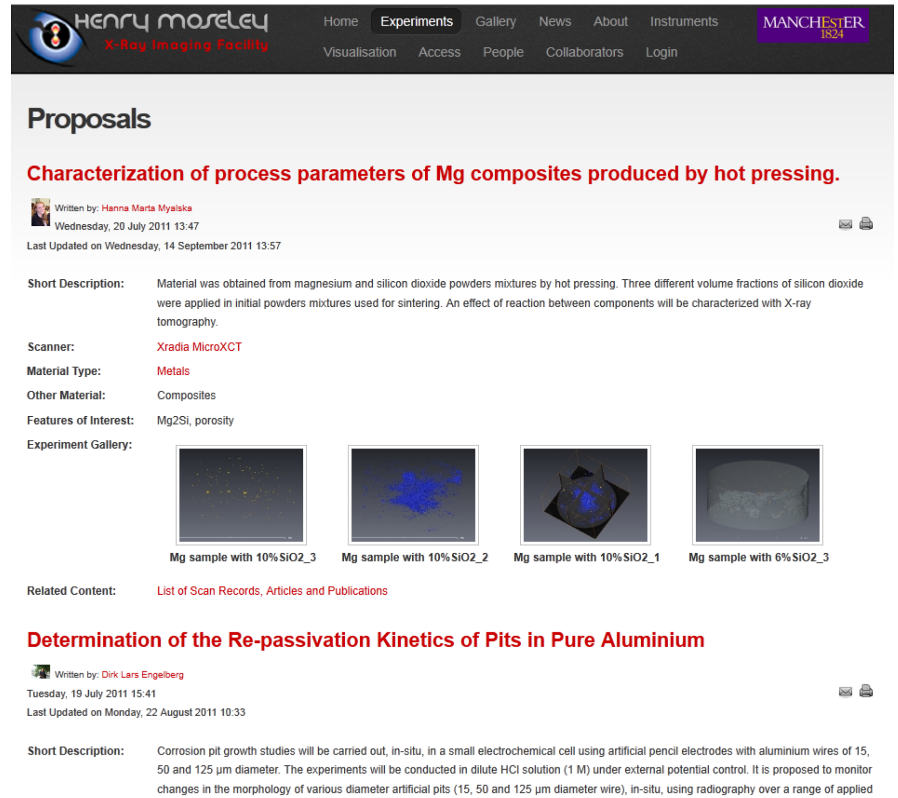
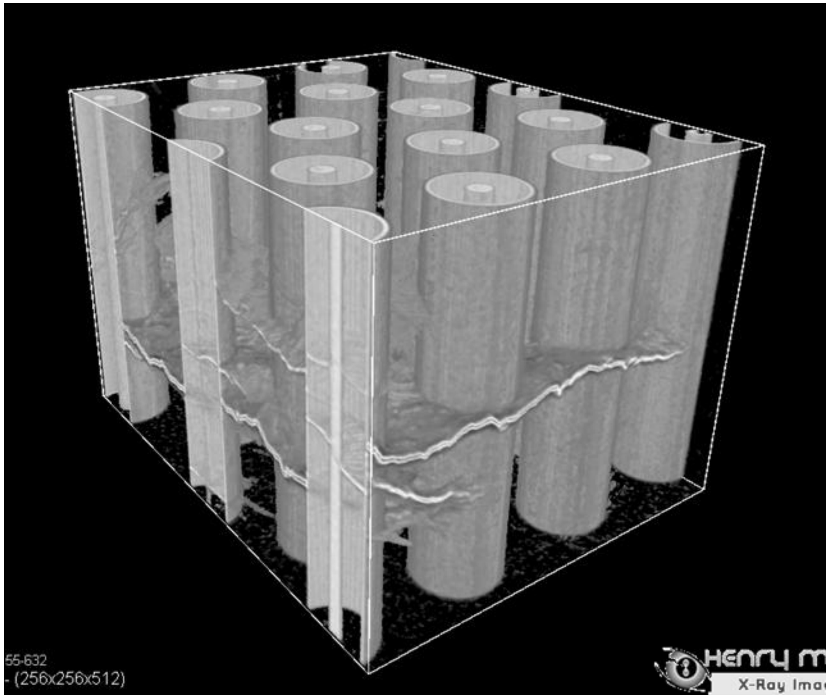
# Experiment Management System



# HMXIF Examples




Incremental crack growth in titanium/silicon carbide

Pacemaker battery

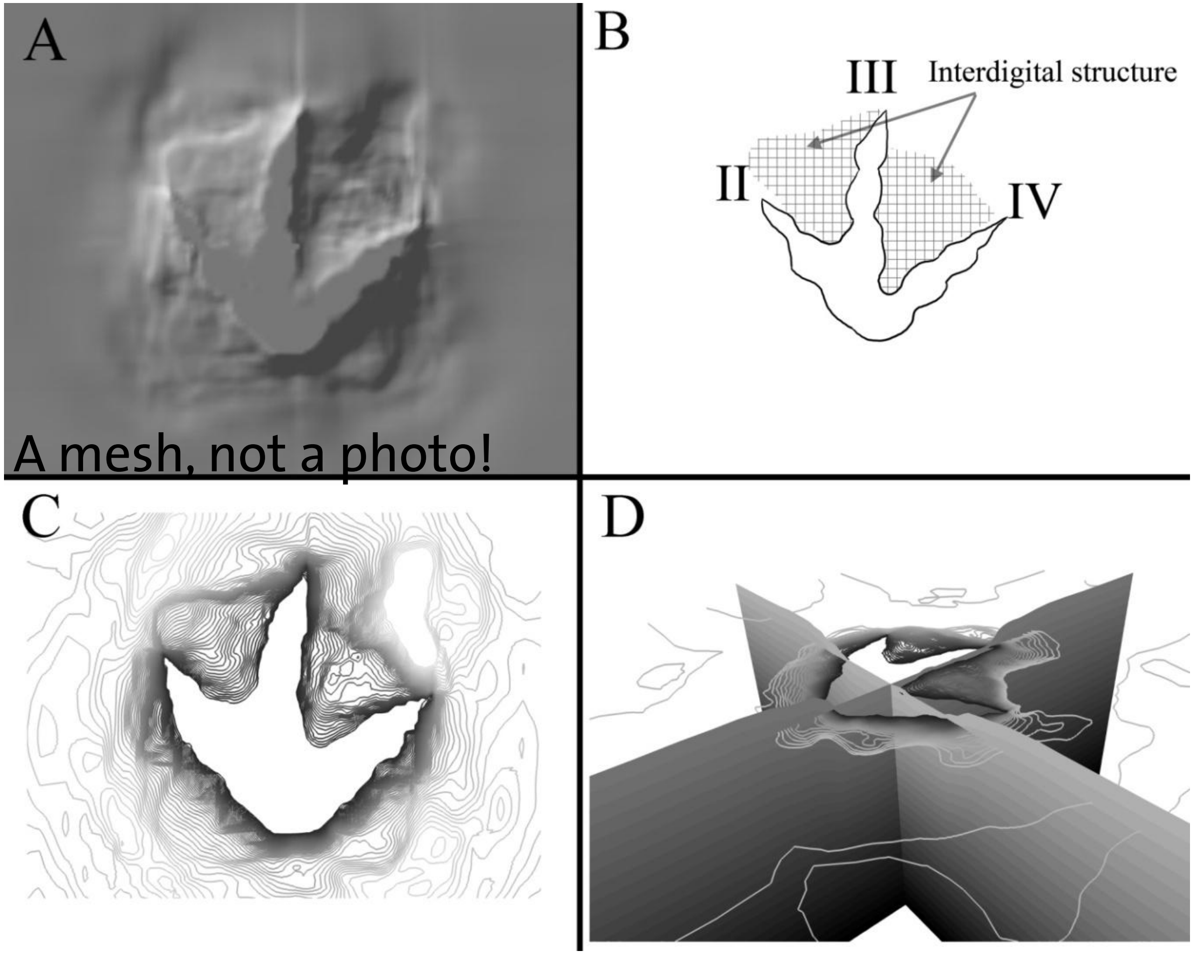
# Imaging

- 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

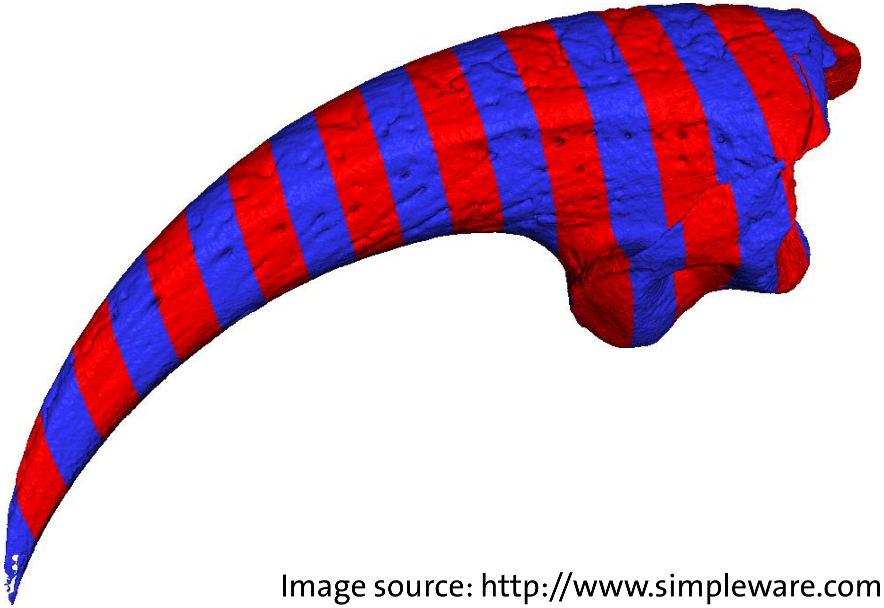


Image source: http://www.simpleware.com

# 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

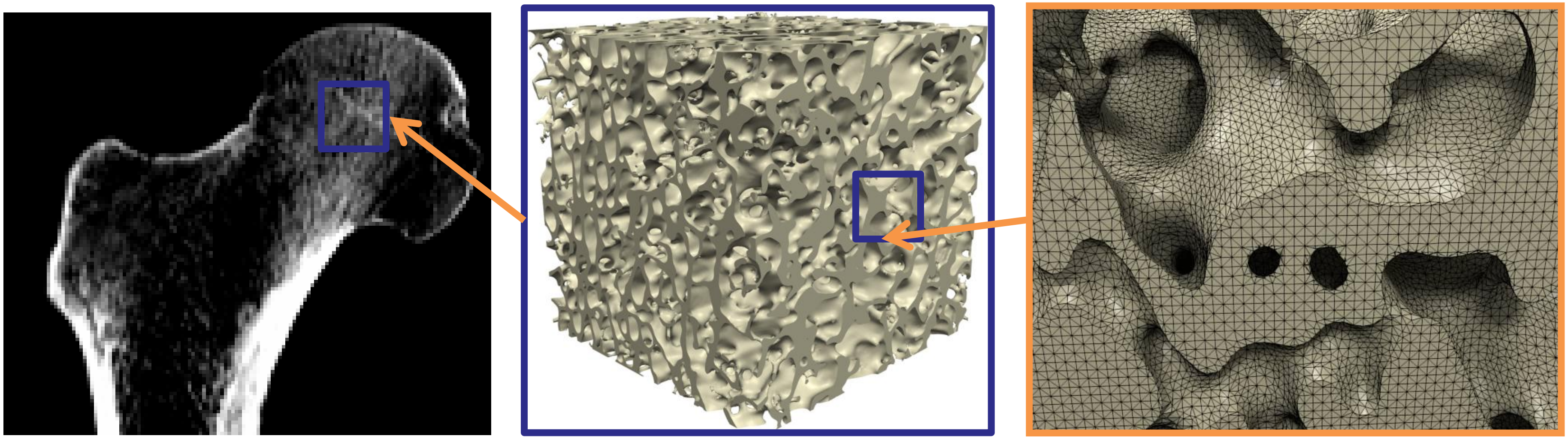


Image source: http://www.simpleware.com

# 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.

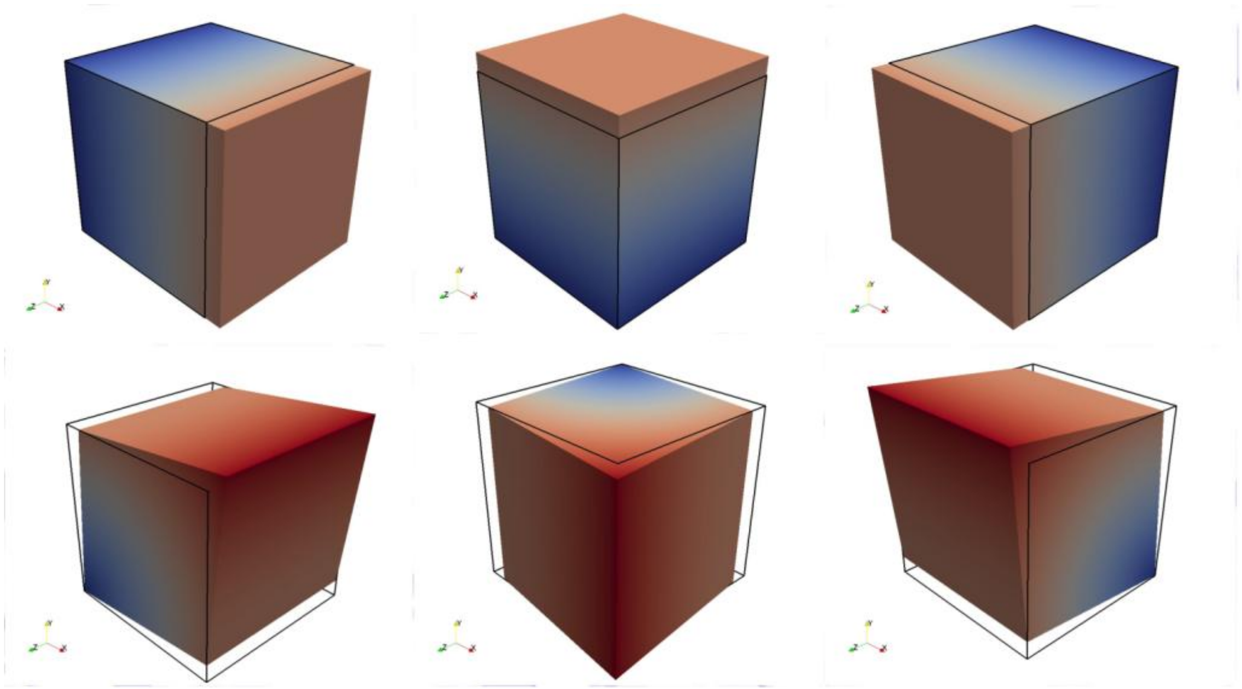


Image source: Peter Falkingham

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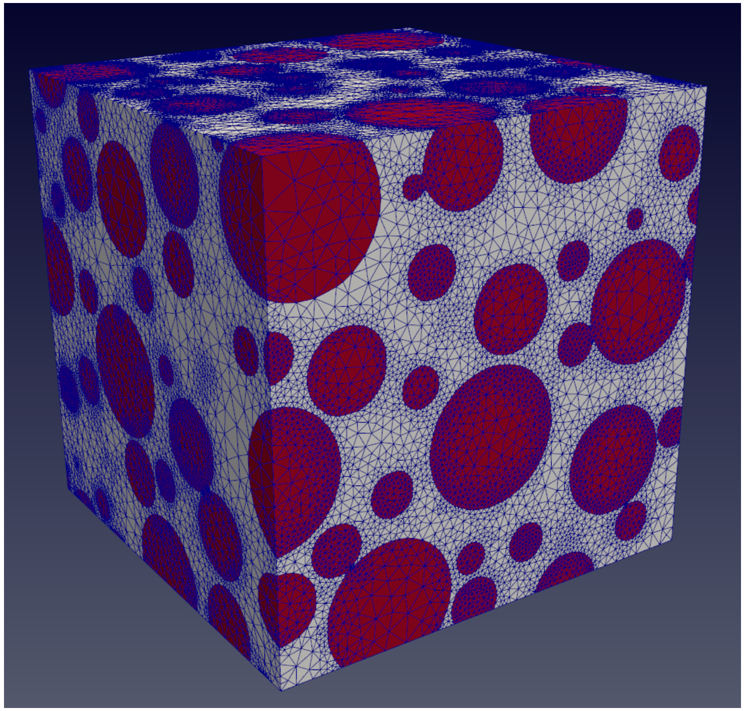
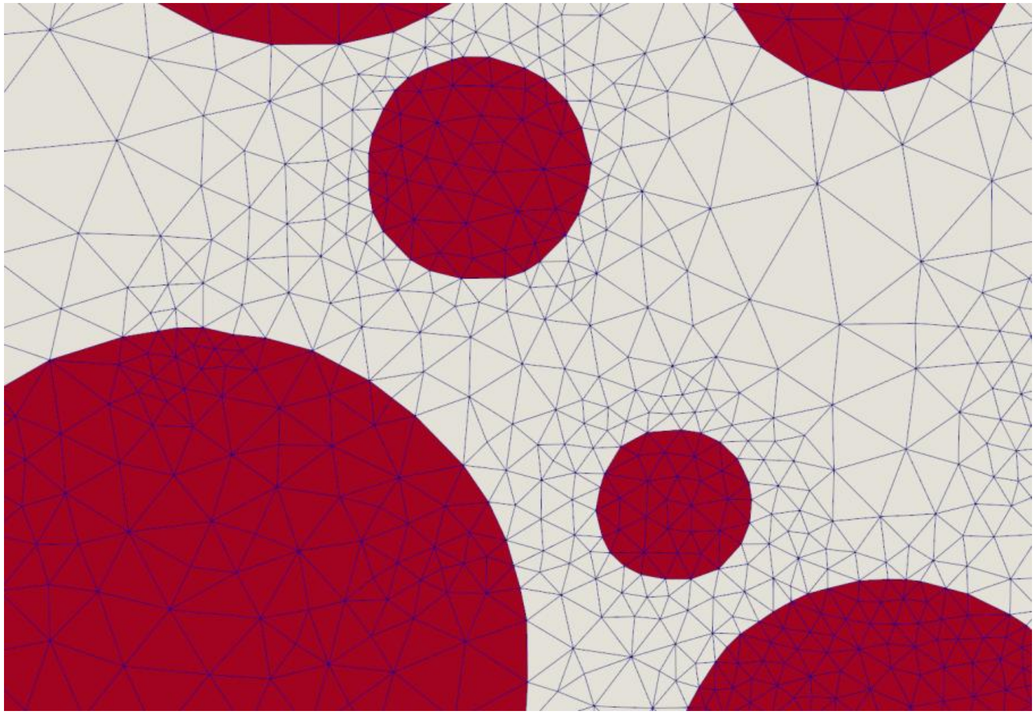
# Multiscale Modelling

## Dr Paul Mummery and Dr Philippe Young

- EDF homogenization benchmark problem
- 330+ million elements

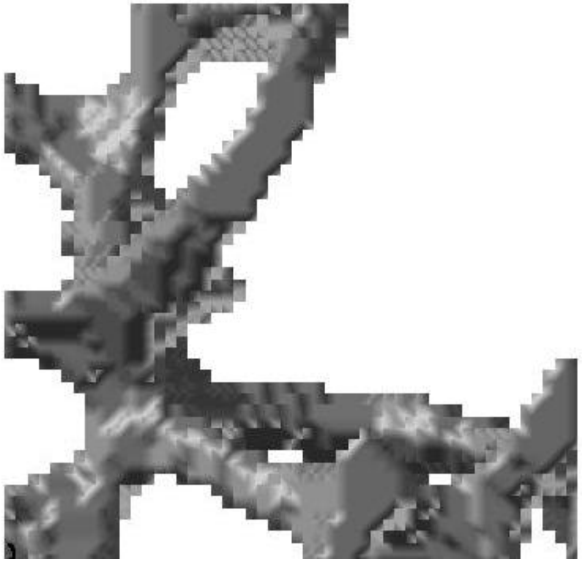




# HECToR GPU Testbed

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

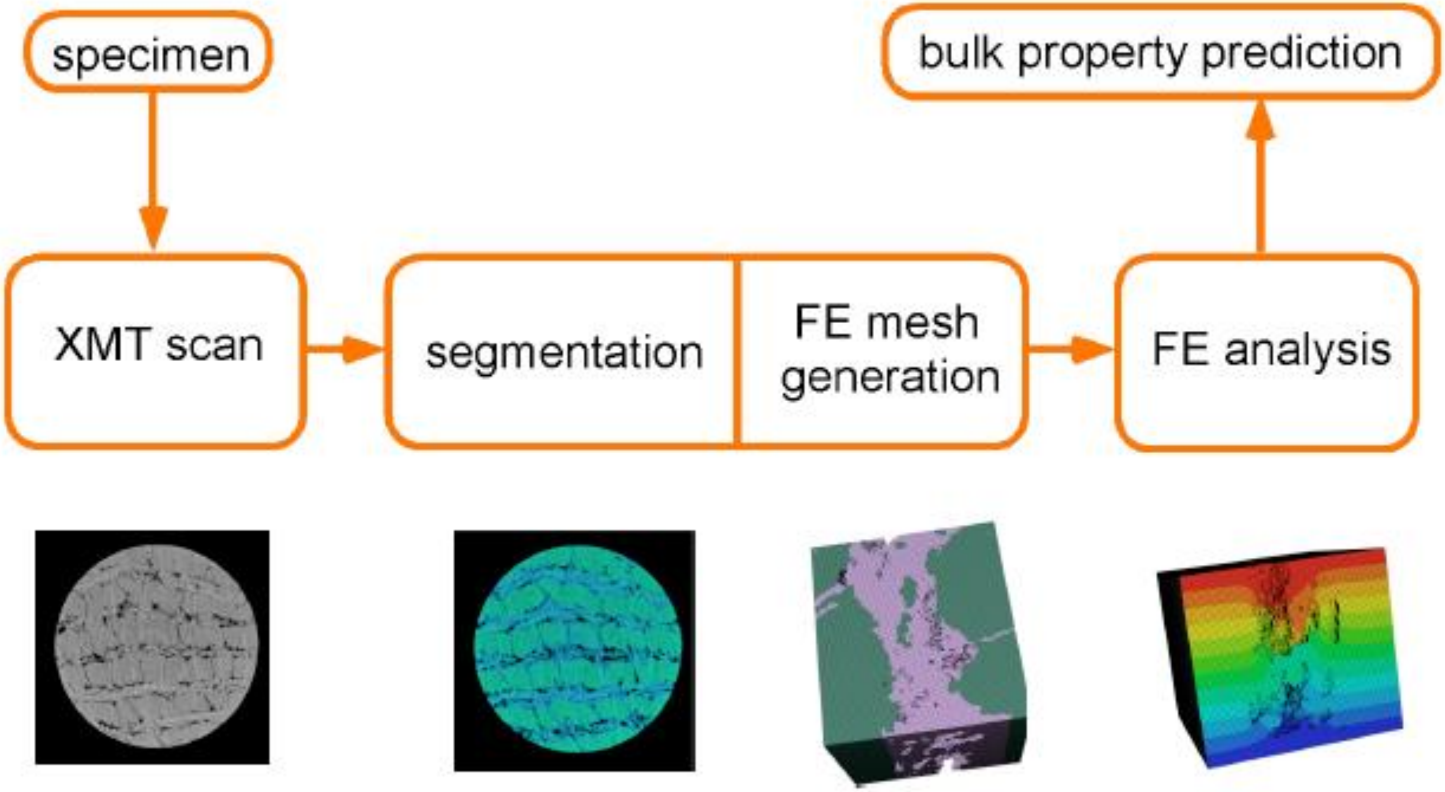


- Some special cases, voxelated meshes from CT images very suitable
- Single matrix, multiple vectors – high level memory reuse

# dCSE Project

# Image Based Modelling

Professor Philip Withers & Professor Paul Mummery



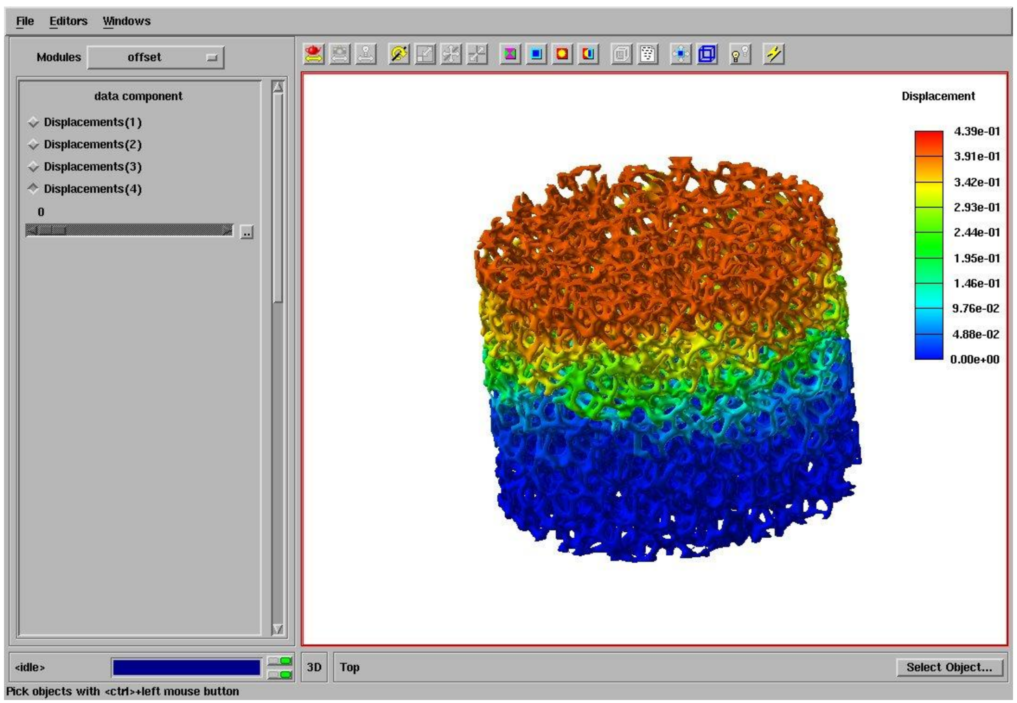

Supporting Henry Moseley X-Ray Imaging Facility

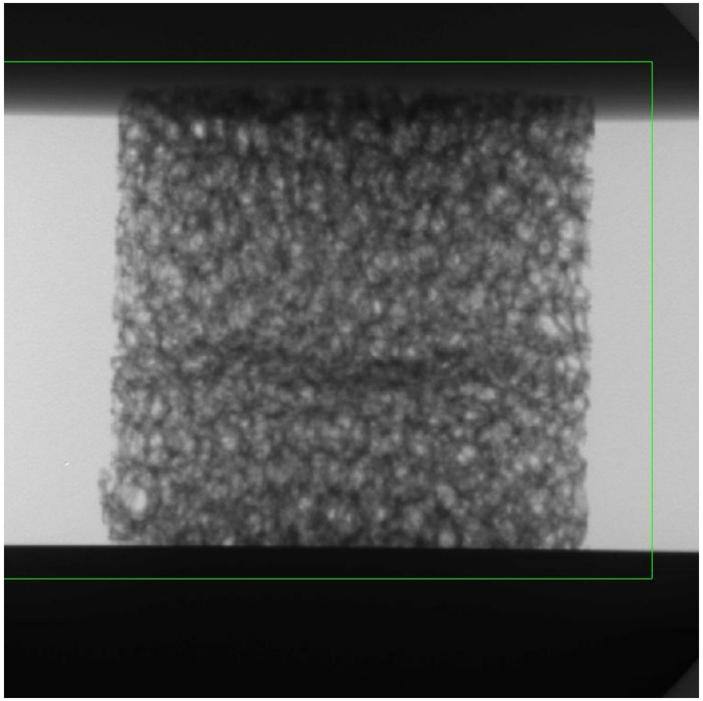
http://xray-imaging.org.uk/

# NAG dCSE

Dr Paul Mummery, Prof Stephane Bordas & Prof Karl Kadler

- 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

# UMAT

- User MAterial 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)

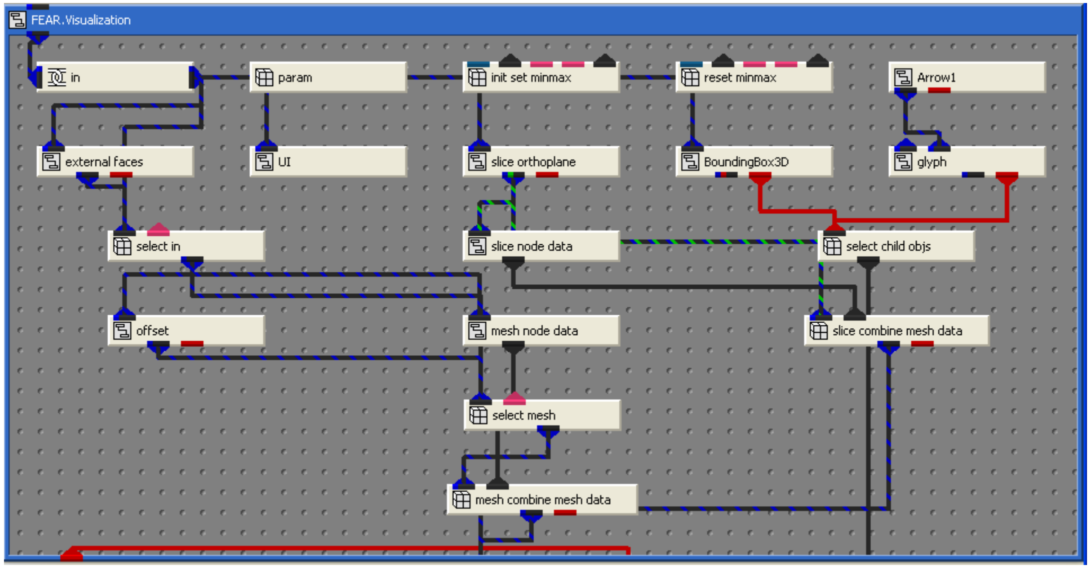
# UMAT Fortran API

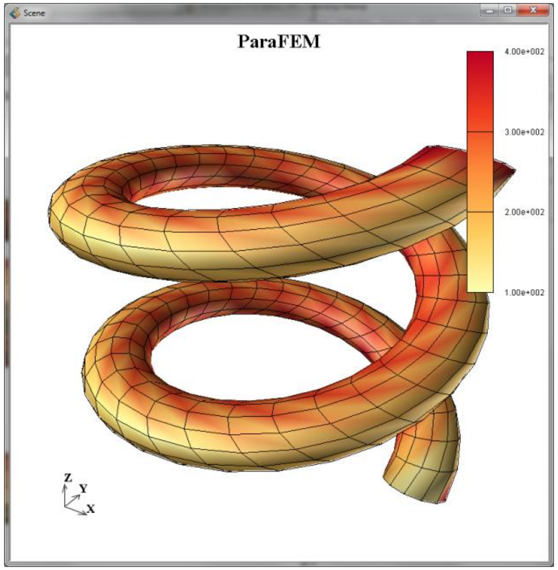
xx1.f90 - parafem - A Portable Librar...

```fortran
!---------------------------------------------------------------------------
! 8. Element stiffness integration and storage
!
!    Note that the DEEMAT and UMAT subroutines are currently outside the loop
!    elements_3. This is only correct when all the elements are of the same
!    type and have the same material properties.
!---------------------------------------------------------------------------

 CALL sample(element,points,weights)

!  dee = zero
!  CALL deemat(e,v,dee)


 dee = zero
 CALL umat(sigma,statev,dee,sse,spd,scd,rpl,ddsddt,drplde,drpldt,stran,      &
           eps,time,dtime,temp,dtemp,predef,dpred,cmname,ndi,nshr,           &
           nst,nstatv,props,nprops,points,drot,pnewdt,celent,dfgrd0,dfgrd1,  &
           iel,npt,layer,kspt,kstep,kinc)

 storkm_pp      = zero

 elements_3: DO iel=1,nels_pp
   gauss_pts_1: DO i=1,nip
     CALL shape_der(der,points,i)
     jac   = MATMUL(der,g_coord_pp(:,:,iel))
     det   = determinant(jac)
     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



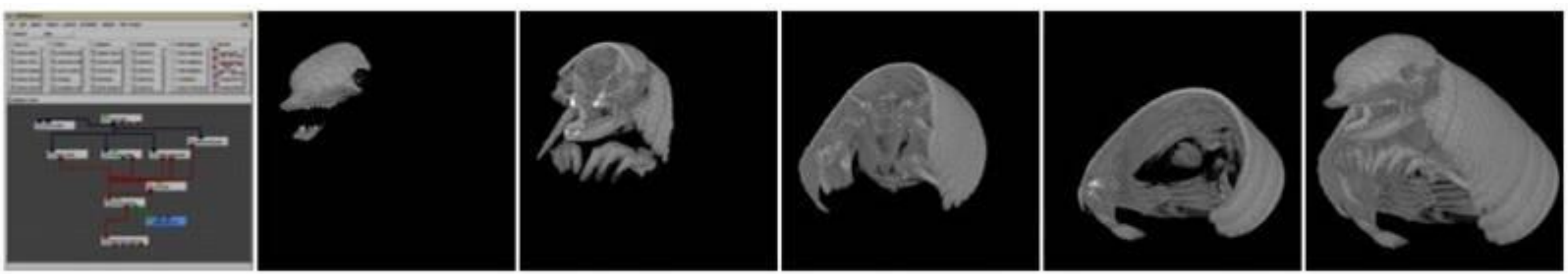



# MRBV

- 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

# MRBV

- 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

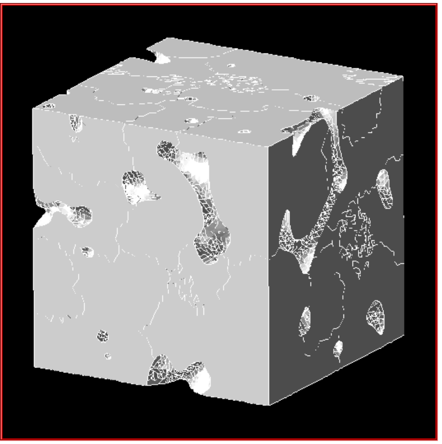
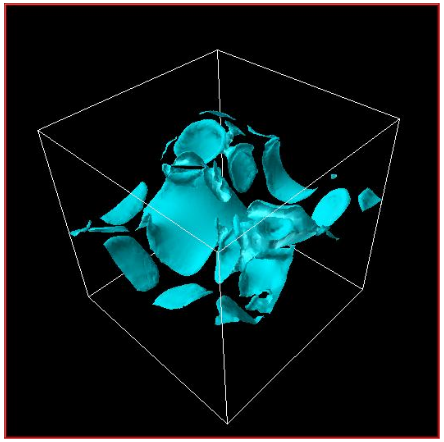
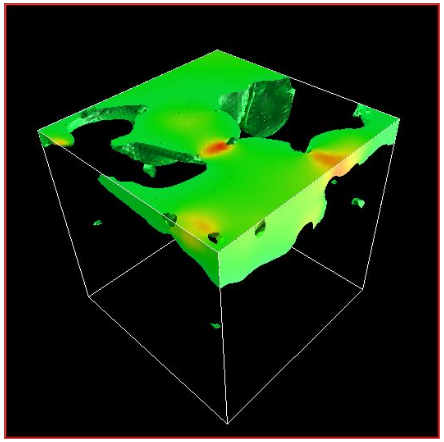
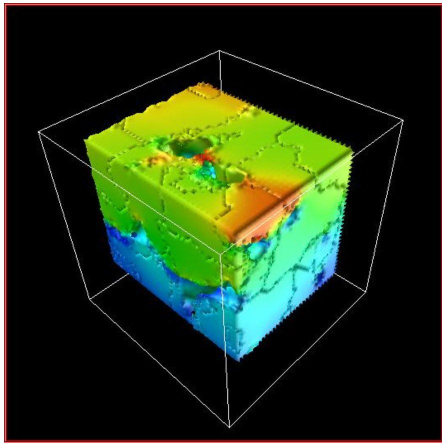


# Porting ParaFEM-Viewer to MRBV

- 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

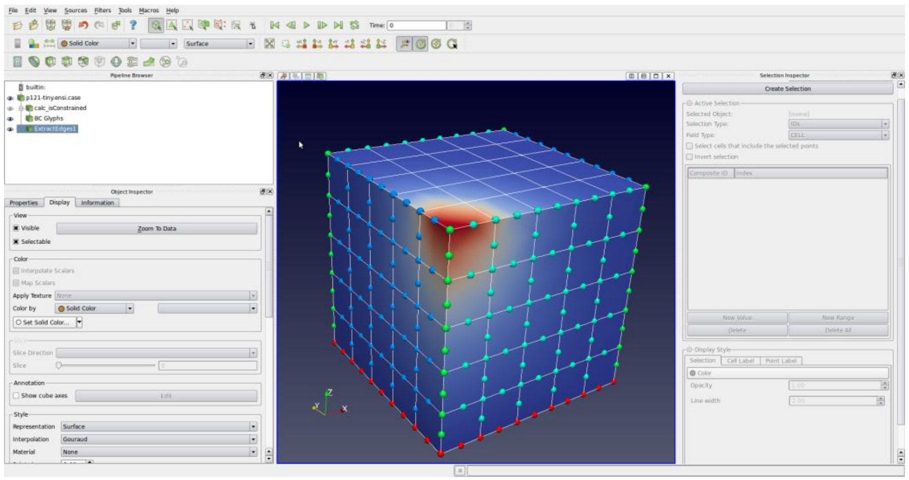
# Using ParaView

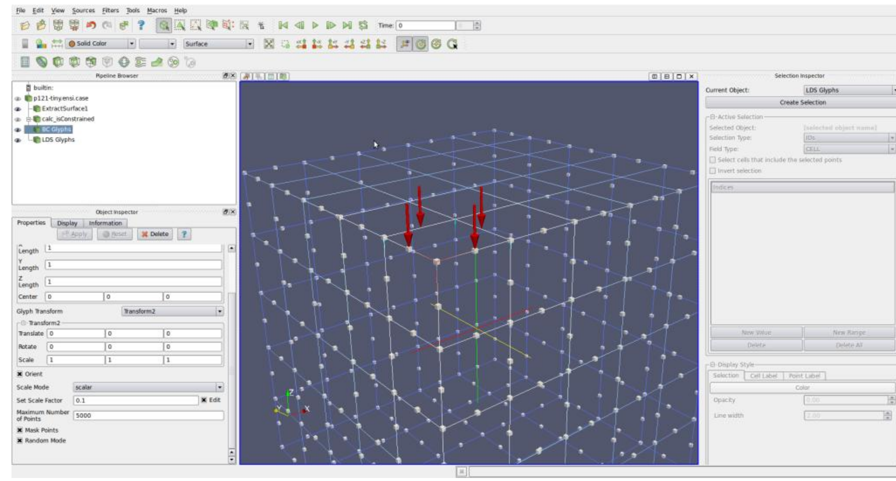
- Benefits
  - Open Source, freely customizable, multi-platform
  - Built on comprehensive and sophisticated VTK library
  - Many visualization and parallelization strategies
- Drawbacks
  - Takes users (initially) back to hands-on control of visualization pipeline
  - Greater effort to provide a custom interface

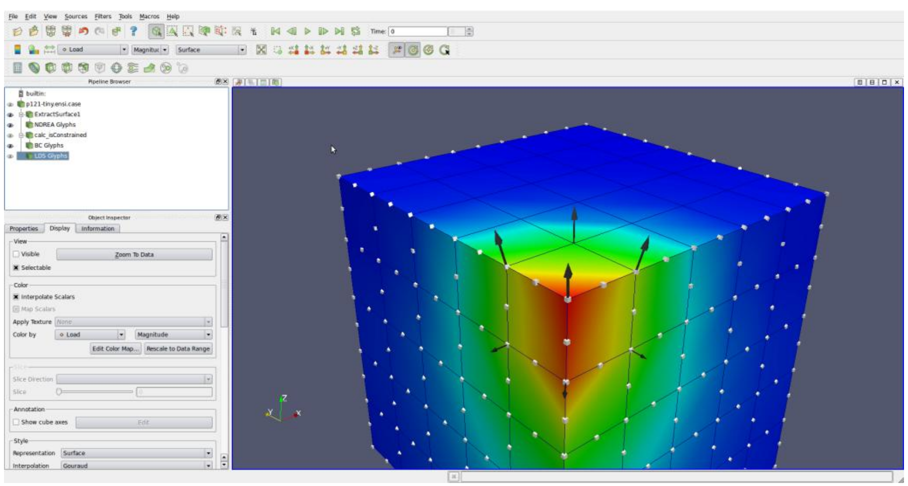
# Moving to ParaView

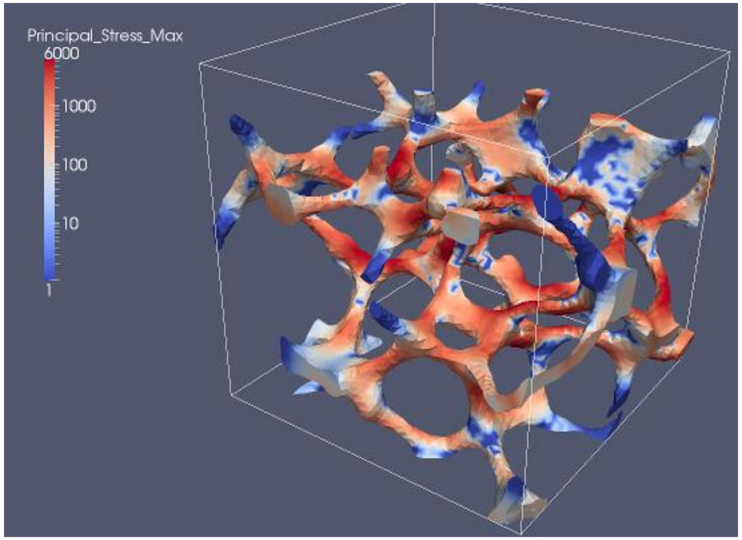
- Data format handling
  - No native ParaFEM reader for ParaView
  - Beyond scope of dCSE project
  - Opted for conversion to supported EnSight Gold Format
- Issues
  - ASCII only at the moment
  - VTK reader code has errors and does not load partial data
  - VTK code fixed but not submitted yet
  -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

# ParaFEM Results in ParaView

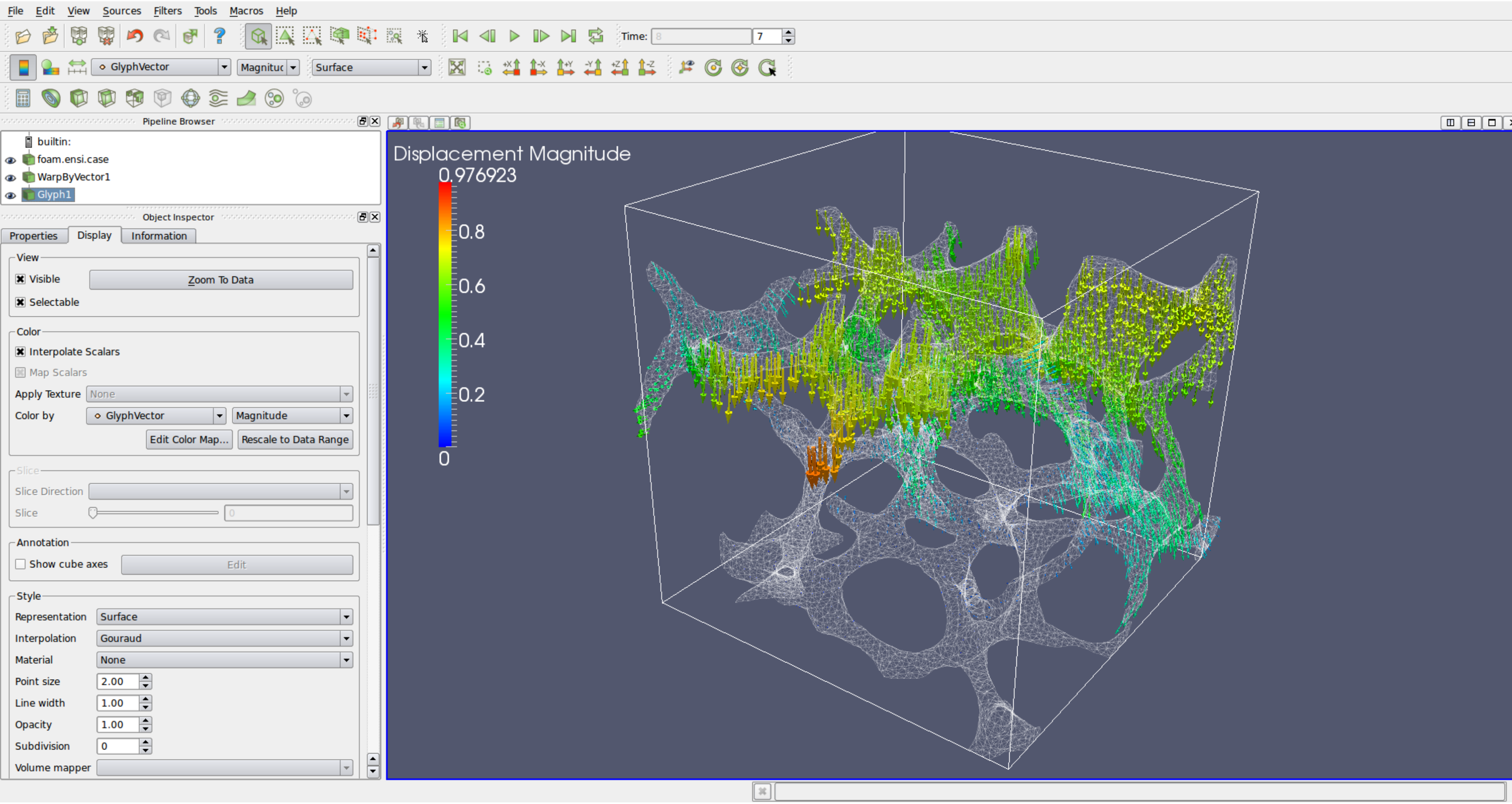








# ParaFEM Results in ParaView

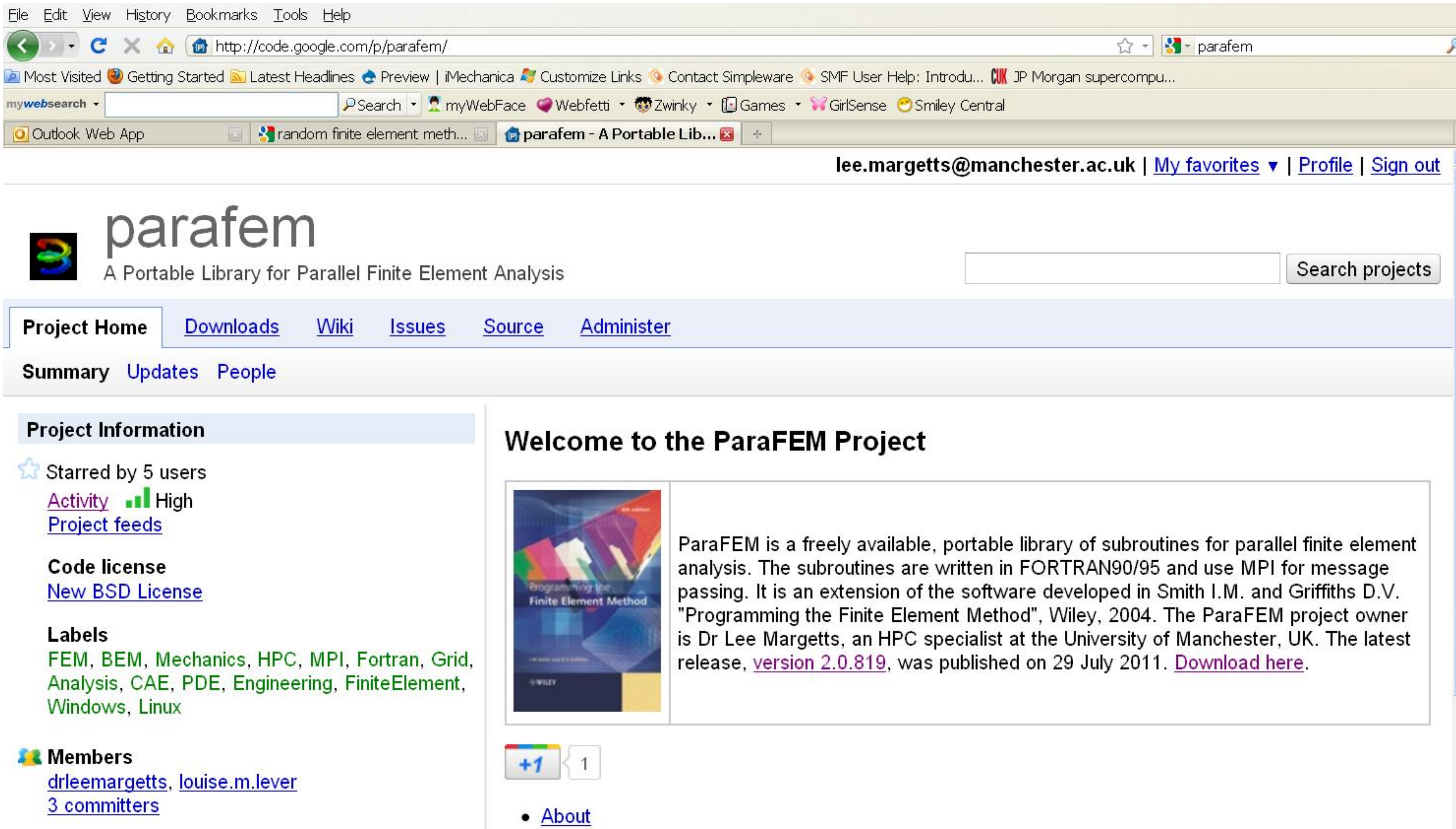


# Remaining Work on dCSE

- 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/parafem/

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parafem

A Portable Library for Parallel Finite Element Analysis

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**Project Information**

Starred by 5 users

Activity High

Project feeds

**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**

Programming the Finite Element Method

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.

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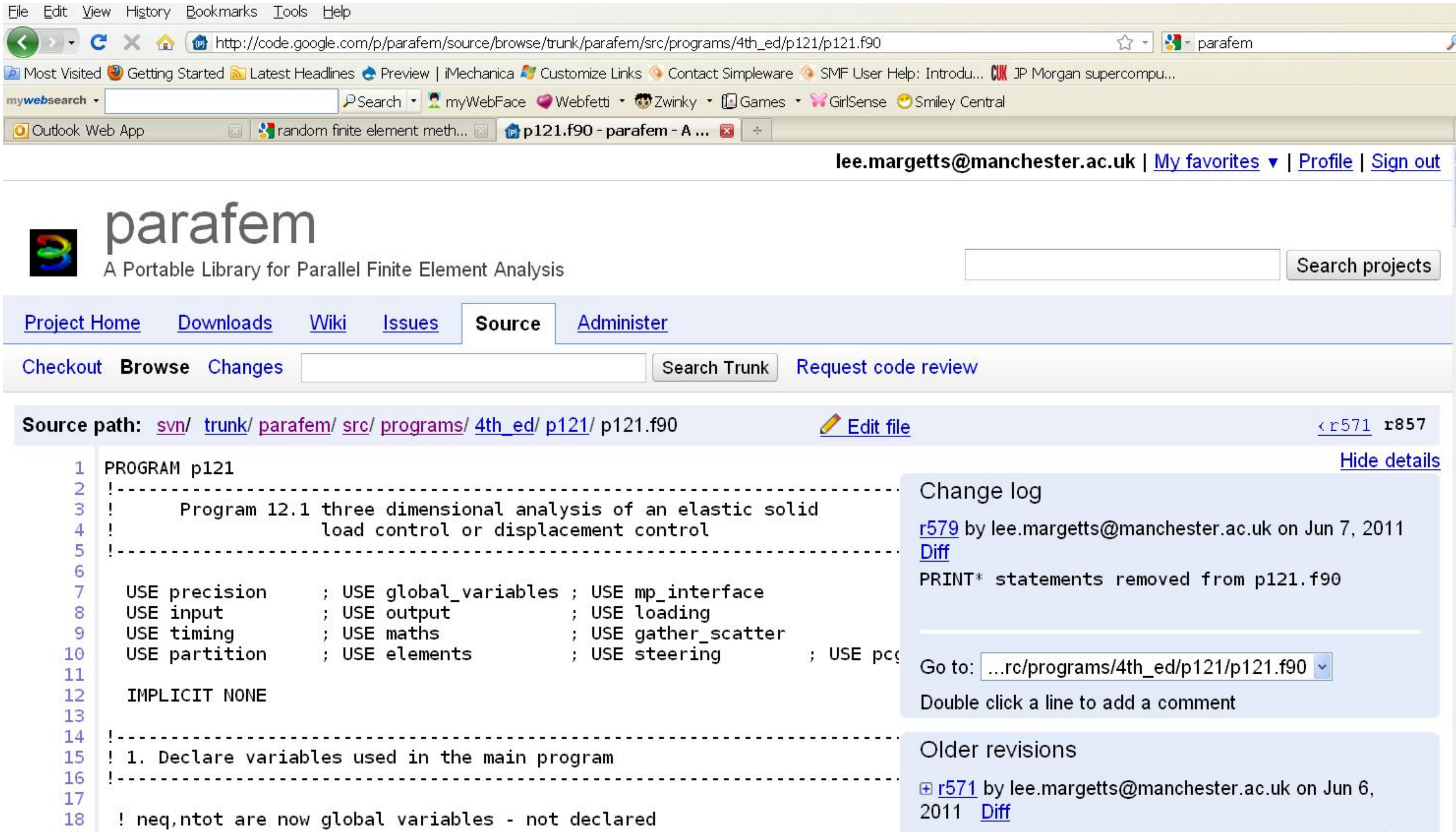
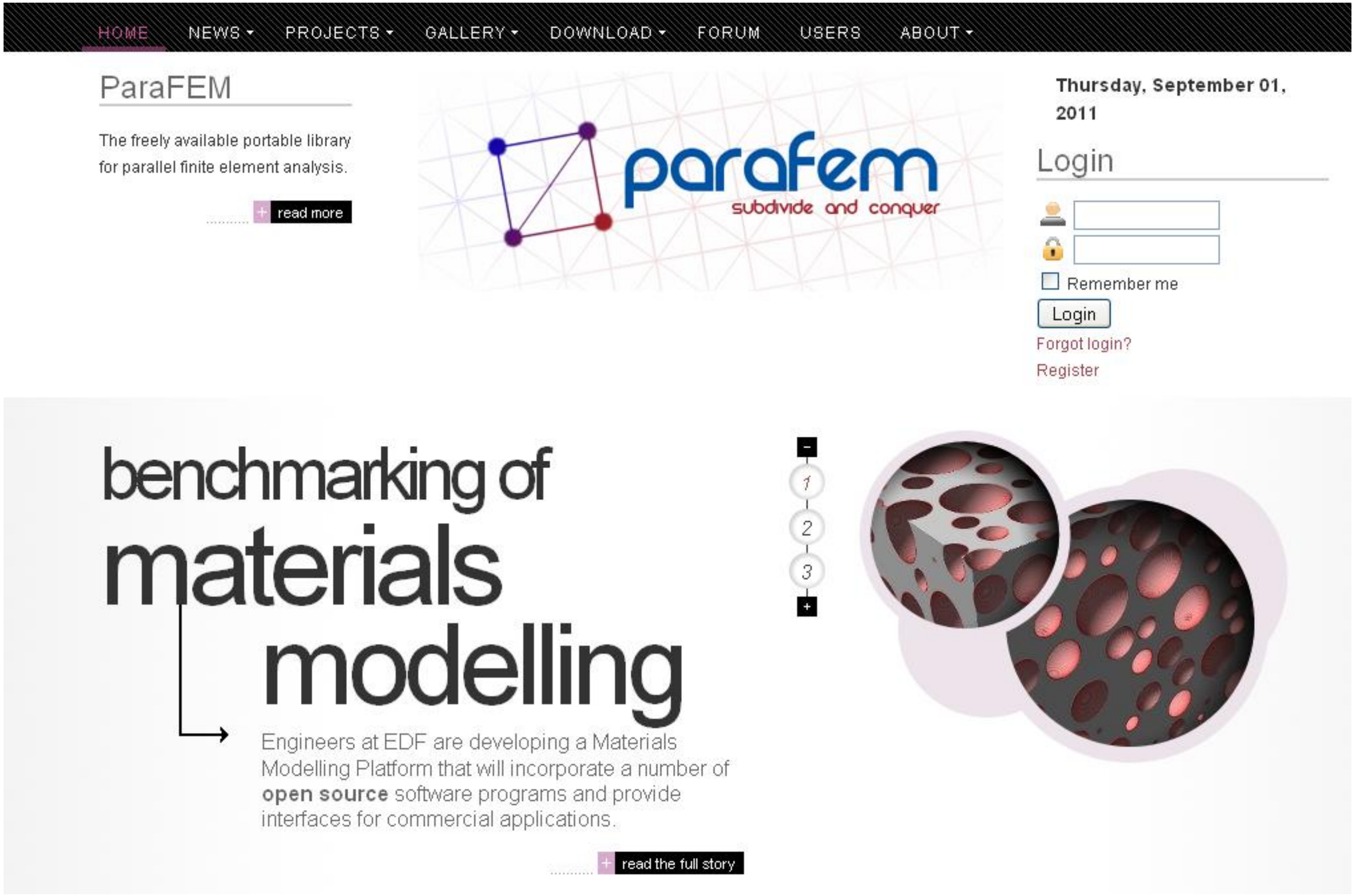
- About

# Google Code Platform



# http:/parafem.org.uk



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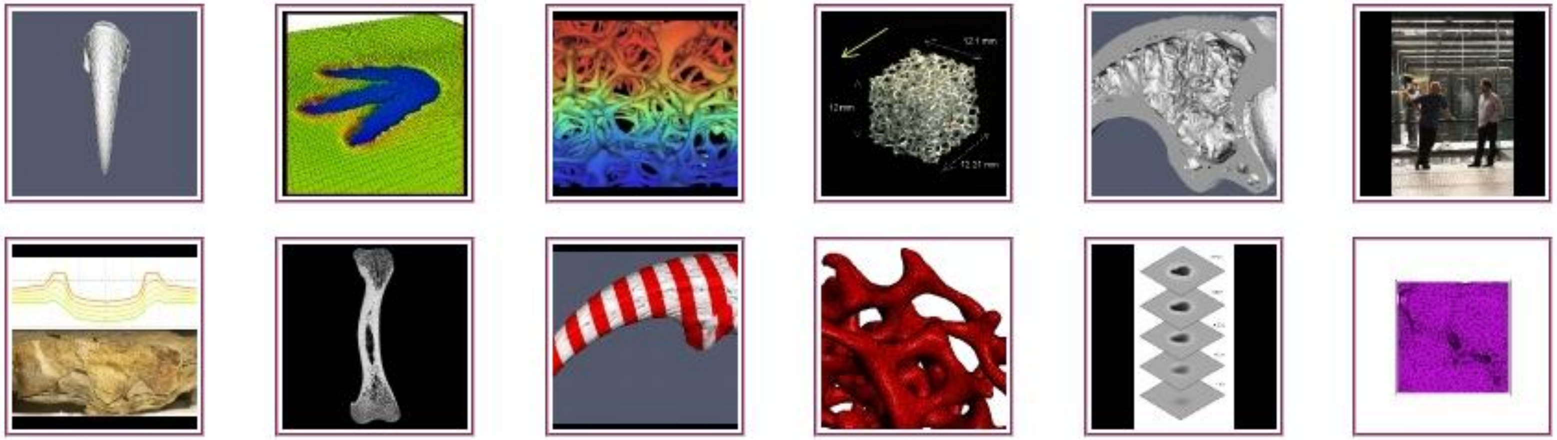
# Joomla Community Building Platform

## 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

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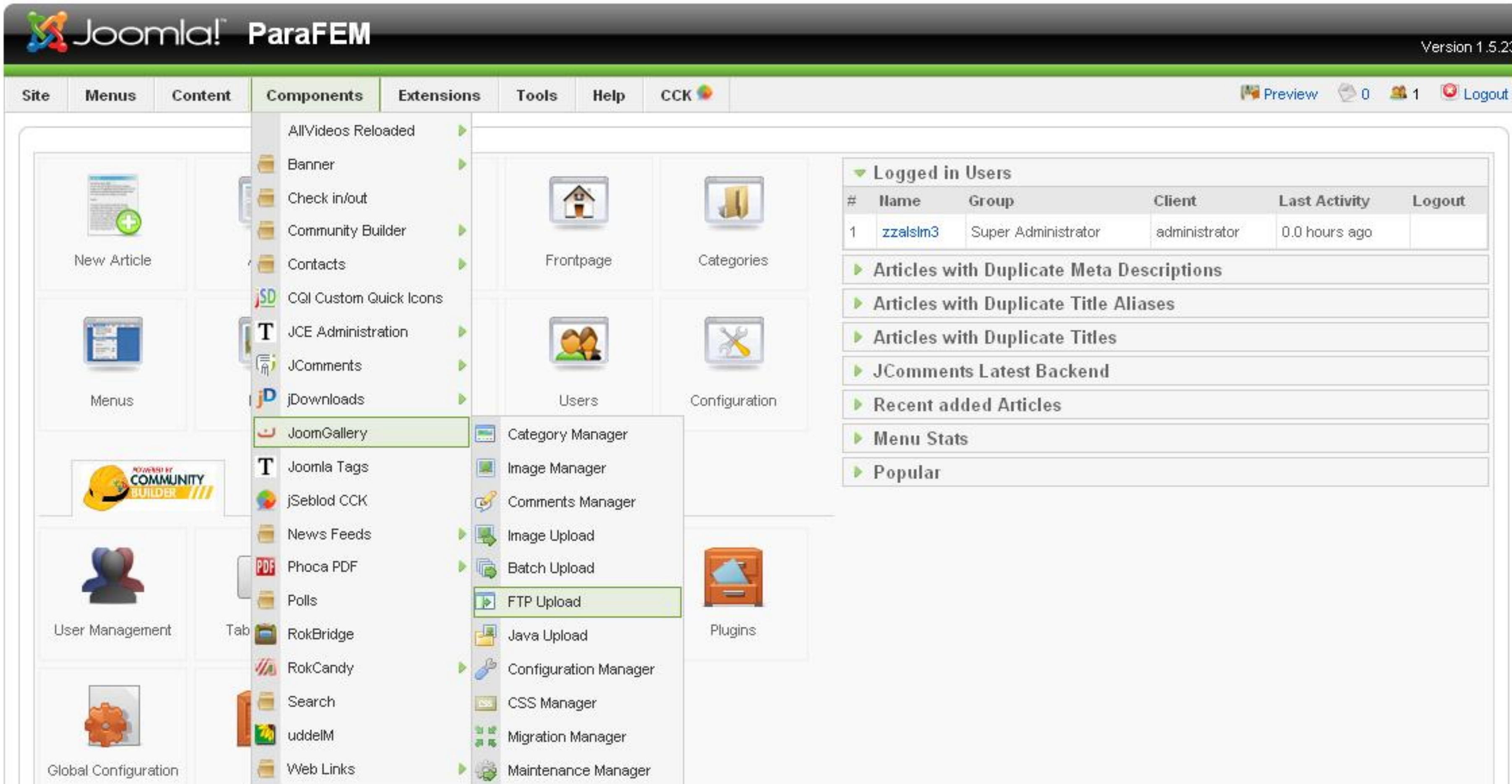
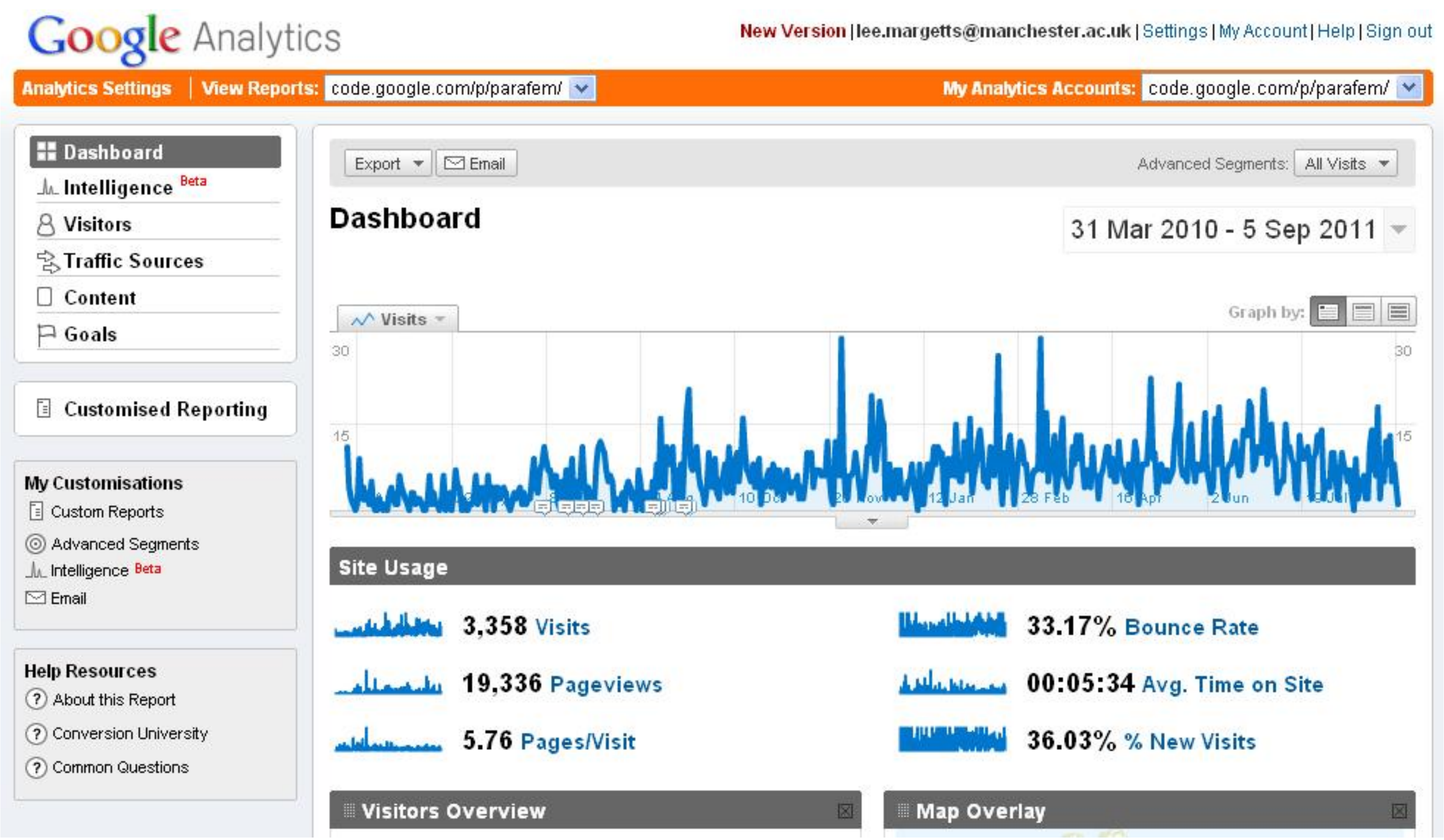
# Joomla back end for parafem.org.uk

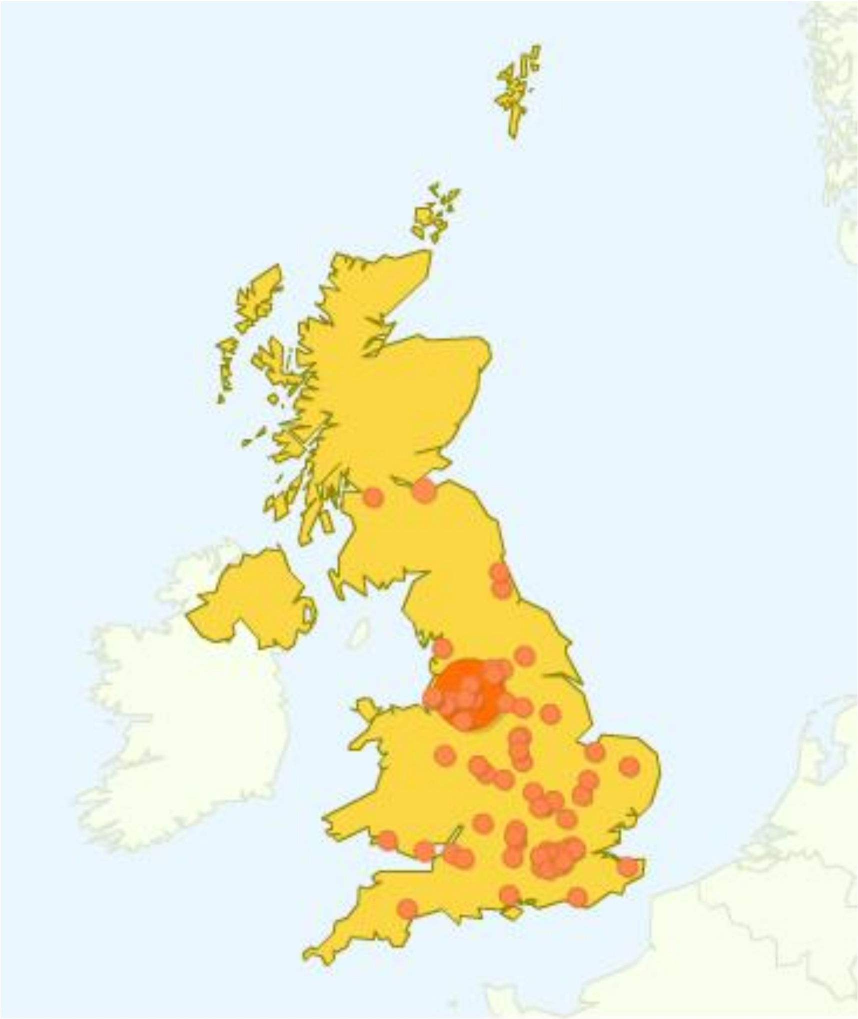


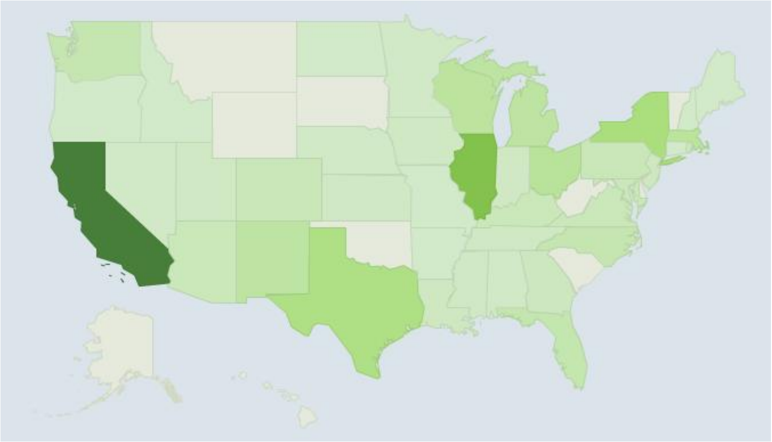
# How well are we doing?



# Visitors - code.google.com/p/parafem

# Visitors - code.google.com/p/parafem





# Acknowledgements

NAG, Dr. Lee Margetts, Prof. Paul Mummery, Prof. Philip Withers, Dr. Phil Manning, Prof. Ian Smith, Dr. Peter Falkingham, Dr. Mohammed Sheikh, Mark Johnson, Dr. David Raymont, Dr. Phillipe Young, Dr. Bill Sellers, Dr. Michael Bane, Vendel Szeremi, Prof. Karl Kadler, George Leaver, Dr. Martin Turner, Dr. Robin Pinning, Dr. Tristan Lowe, Dr. Sam McDonald

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