Future prospects for fatigue modeling on massively parallel computing platforms

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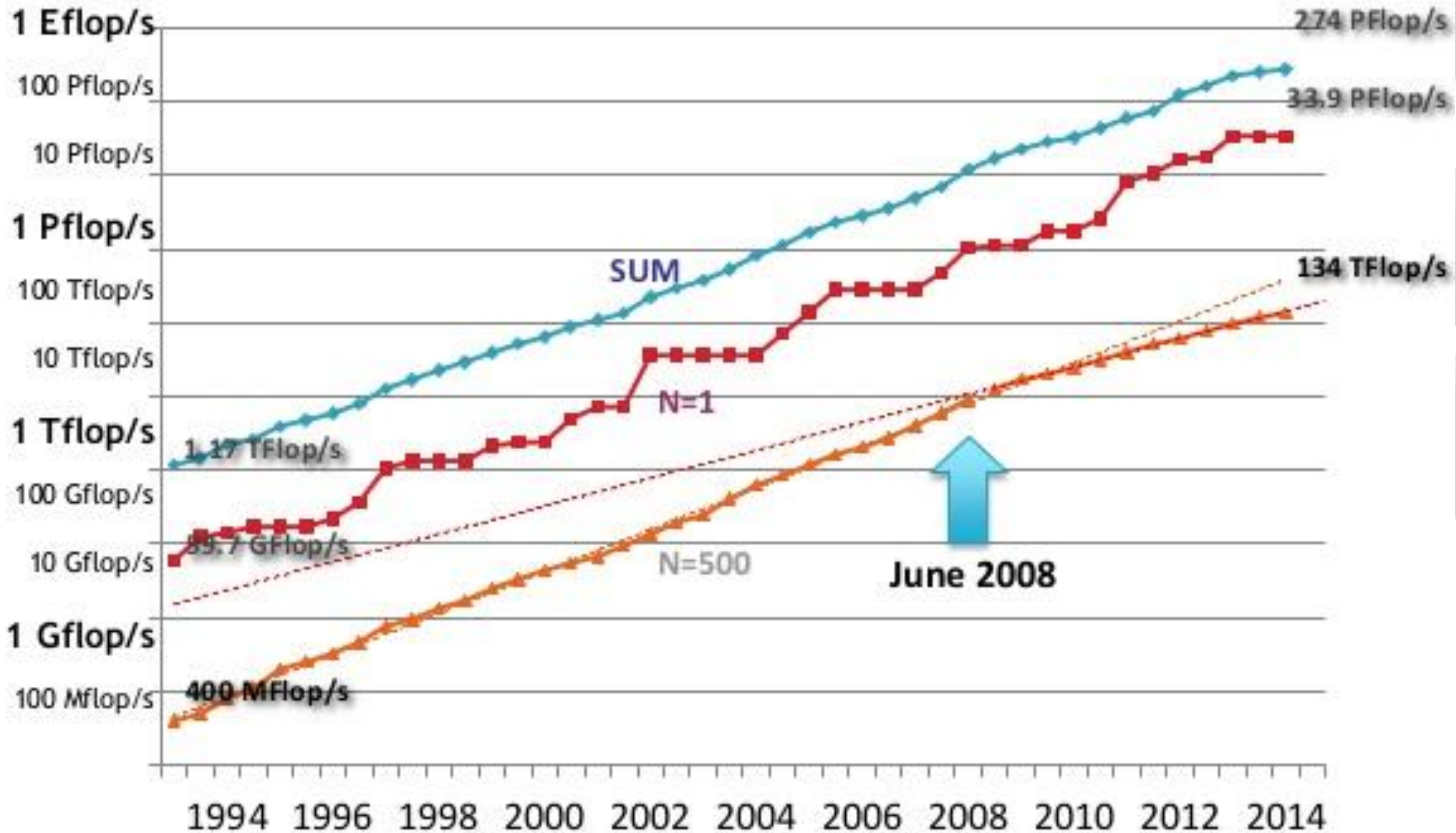
NAFEMS

Overview

- Advances in hardware
  - Parallel processing
- 4D Imaging
  - Fatigue and fracture surfaces
- Multiscale modelling
  - Mechanistic vs phenomenological
- Summary
- References

Advances in Hardware

Performance Development



TOP500 SUPERCOMPUTER SITES

Titan, Oak Ridge National Laboratory
20+ Petaflops

299,008 cores (Opteron) and 18,600 NVIDIA GPUs

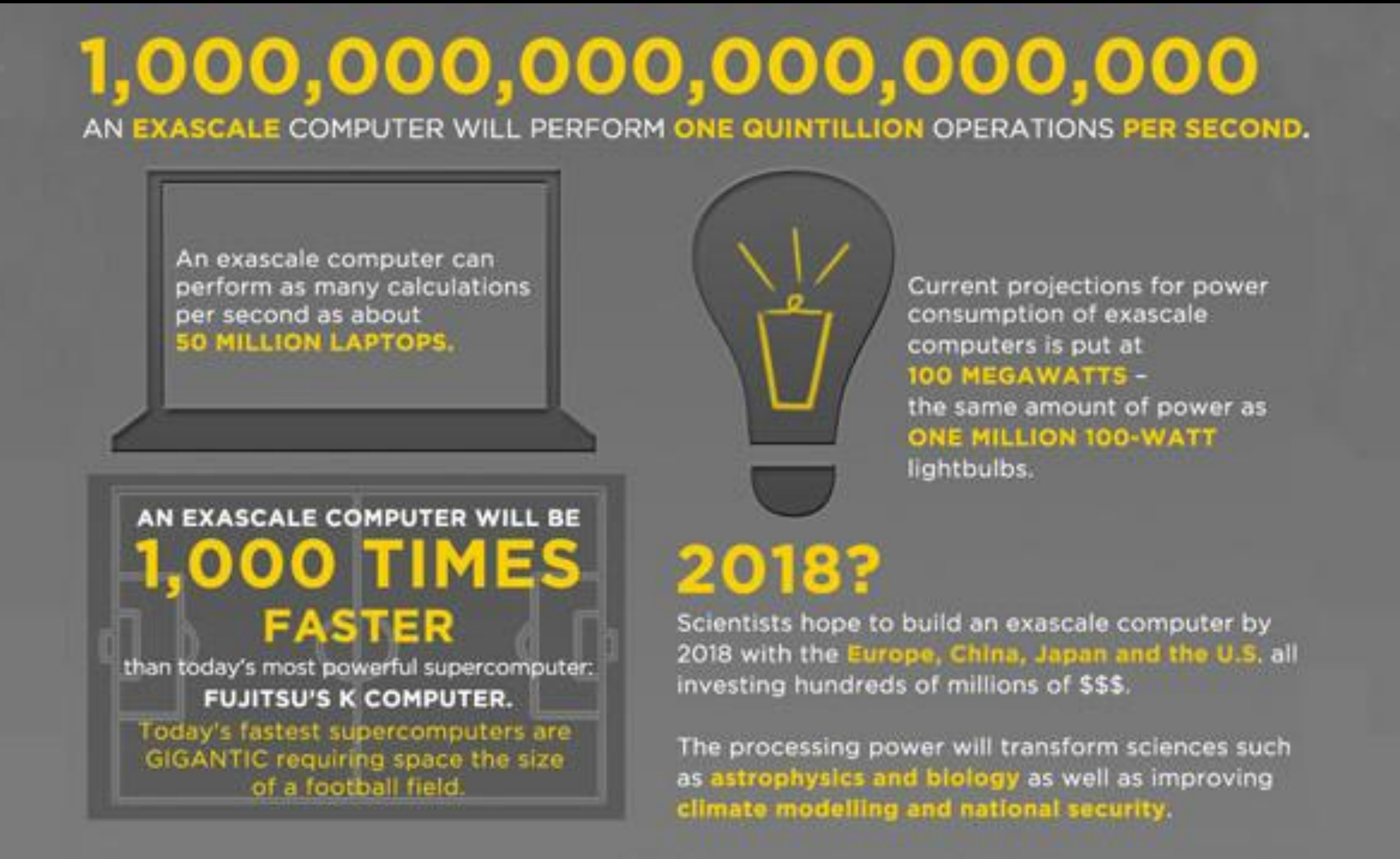
>20,000,000,000,000,000 floating point operations per second

Tianhe-2

33.86 Petaflops

3,120,000 cores (Intel Ivy Bridge and Xeon Phi)

33,860,000,000,000,000 floating point operations per second


1,000,000,000,000,000,000
AN EXASCALE COMPUTER WILL PERFORM ONE QUINTILLION OPERATIONS PER SECOND.
An exascale computer can perform as many calculations per second as about 50 MILLION LAPTOPS.
Current projections for power consumption of exascale computers is put at 100 MEGAWATTS – the same amount of power as ONE MILLION 100-WATT lightbulbs.
AN EXASCALE COMPUTER WILL BE
1,000 TIMES
FASTER
than today's most powerful supercomputer:
FUJITSU'S K COMPUTER.
Today's fastest supercomputers are GIGANTIC requiring space the size of a football field.
2018?
Scientists hope to build an exascale computer by 2018 with the Europe, China, Japan and the U.S. all investing hundreds of millions of $$$.
The processing power will transform sciences such as astrophysics and biology as well as improving climate modelling and national security.

#1 in 1996?

A8 Processor SoC
~172GFlops?

http://larreks.deviantart.com/art/Evolution-of-Tomb-Raider-425582963

ParaFEM – http//parafem.org.uk

- ParaFEM is a freely available, portable library of subroutines for parallel finite element analysis.
- Written in “Modern” FORTRAN. Uses MPI for message passing.
  - Static Linear Elastic Equilibrium (Small Strain)
  - Static Elasto-plastic Equilibrium
  - Steady State Heat Flow & Seepage (Poisson equation)
  - Steady Fluid Flow (Navier-Stokes equations)
  - Large Strain Elasticity (St Venant-Kirchoff Material)
  - Explicit/Implicit Transient Flow
  - Coupled Transient Deformation/Flow
  - Dynamic Equilibrium of Elastic/Elastoplastic Solids
  - Eigenvalues/vectors (elastic solids)

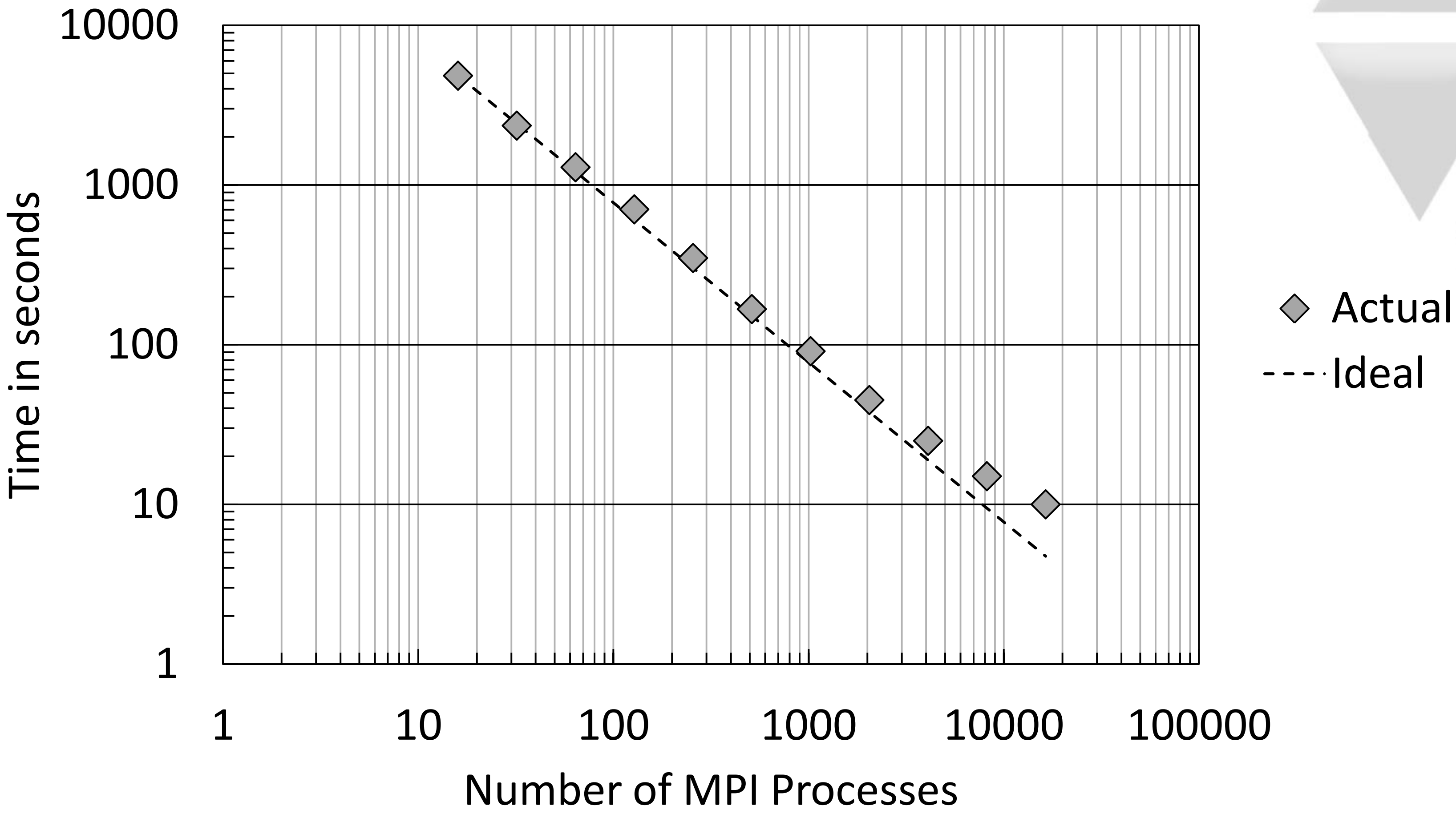
Large FE problems

Mesh Subdivision	Number of Equations
10 x 10 x 10	12,580
20 x 20 x 20	98,360
40 x 40 x 40	777,520
80 x 80 x 80	6,182,240
100 x 100 x 100	12,059,800
400 x 400 x 400	768,959,200
440 x 440 x 440	1,023,368,720

Time for one step

Mesh (equations)	Processes	Time (secs)
12,059,800	16	486
	32	256
	64	140
	128	83
768,959,200	1024	2721
	2048	1213
	4096	662

Scaling one step (125M dof)

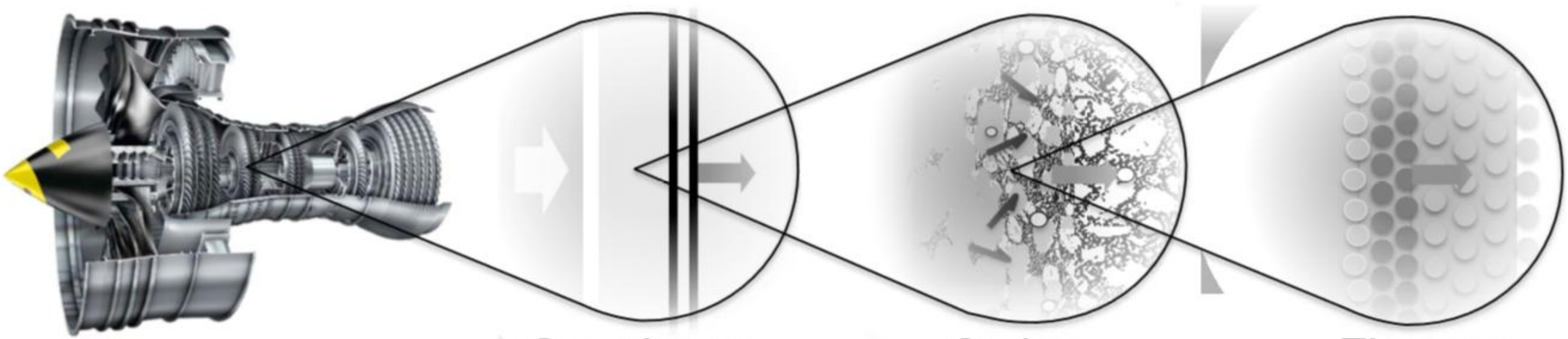


4D Imaging

Fatigue

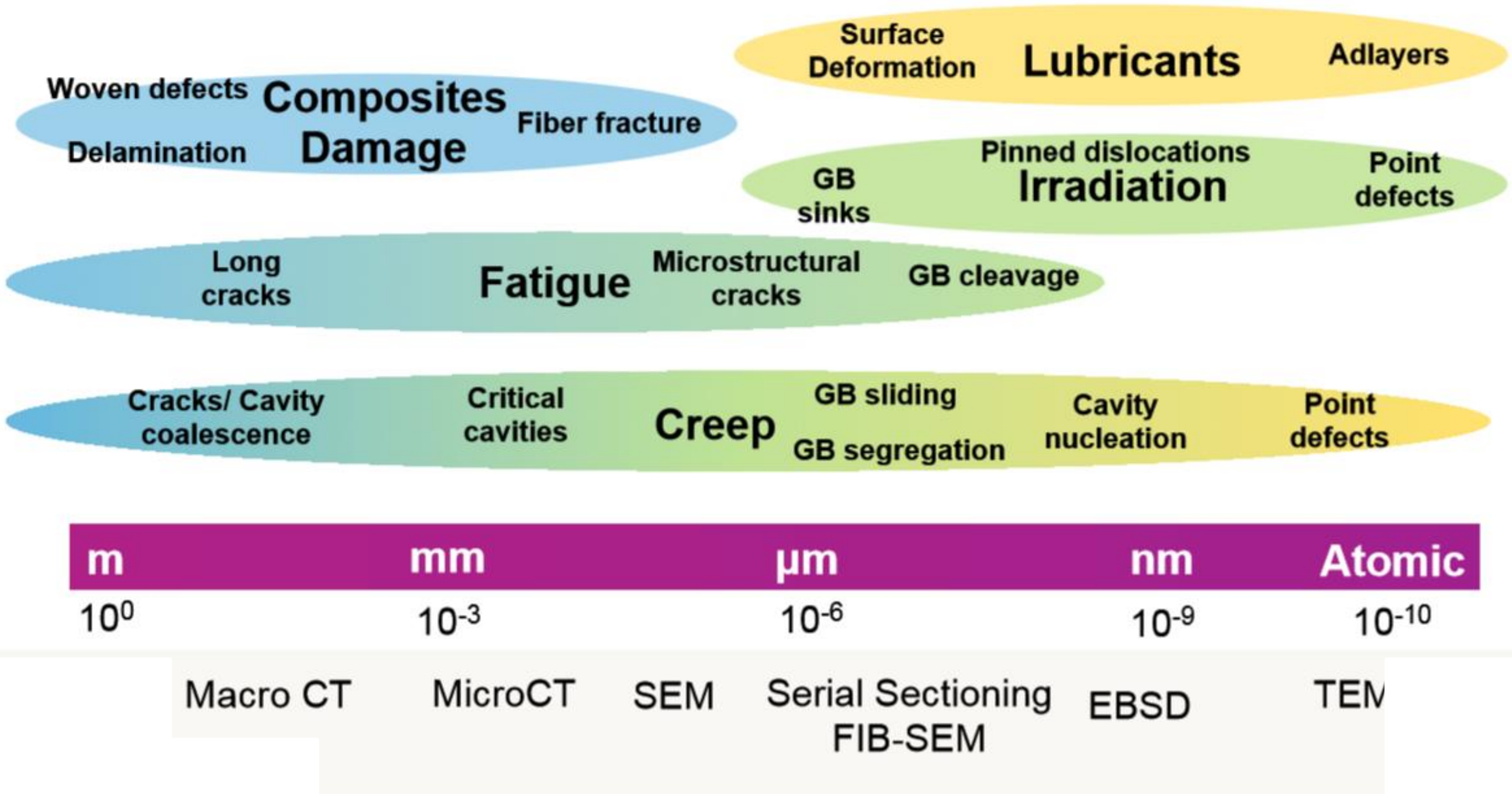
- Weakening of a material caused by repeatedly applied loads.
- Progressive and localized structural damage.
- Microscopic cracks form at stress concentrators such as the surface, persistent slip bands and grain interfaces

Scales in condensed matter

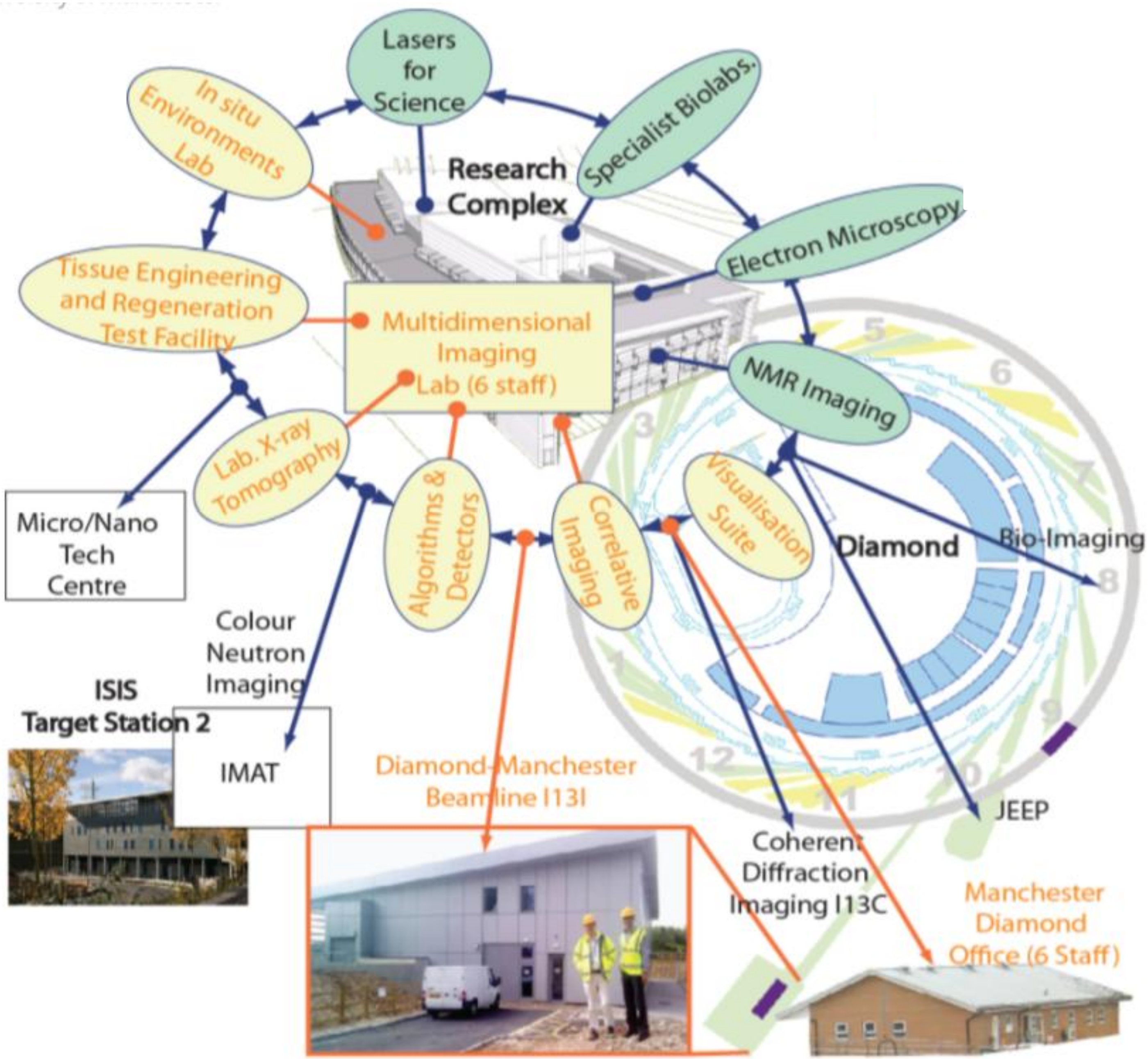


Source: Professor Neil Bourne

Imaging techniques



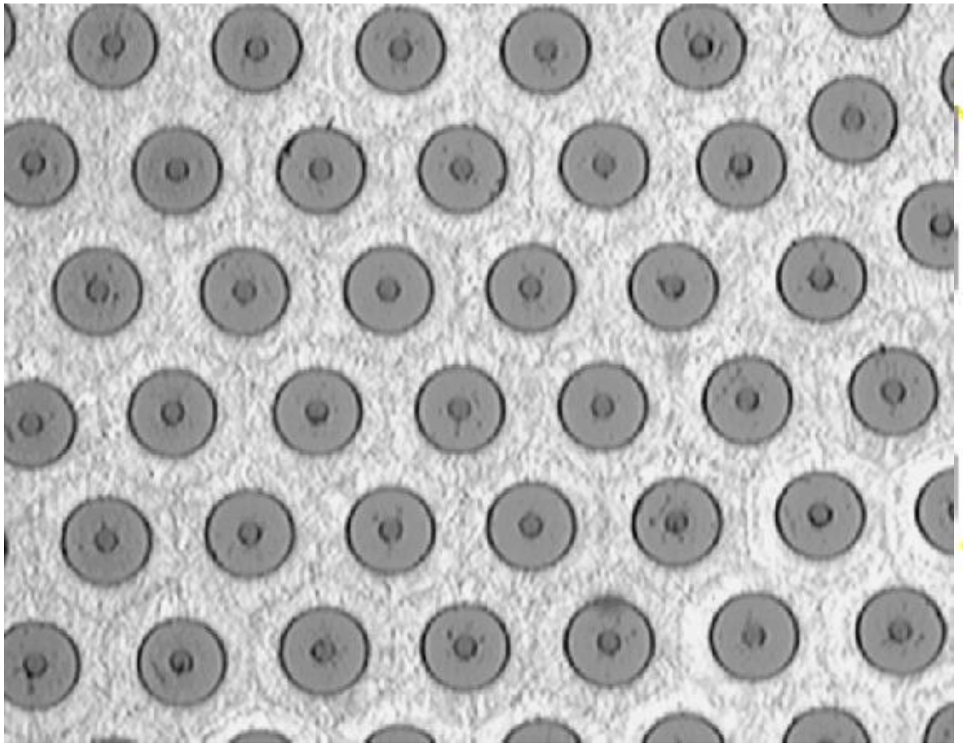
Source: Professor Neil Bourne



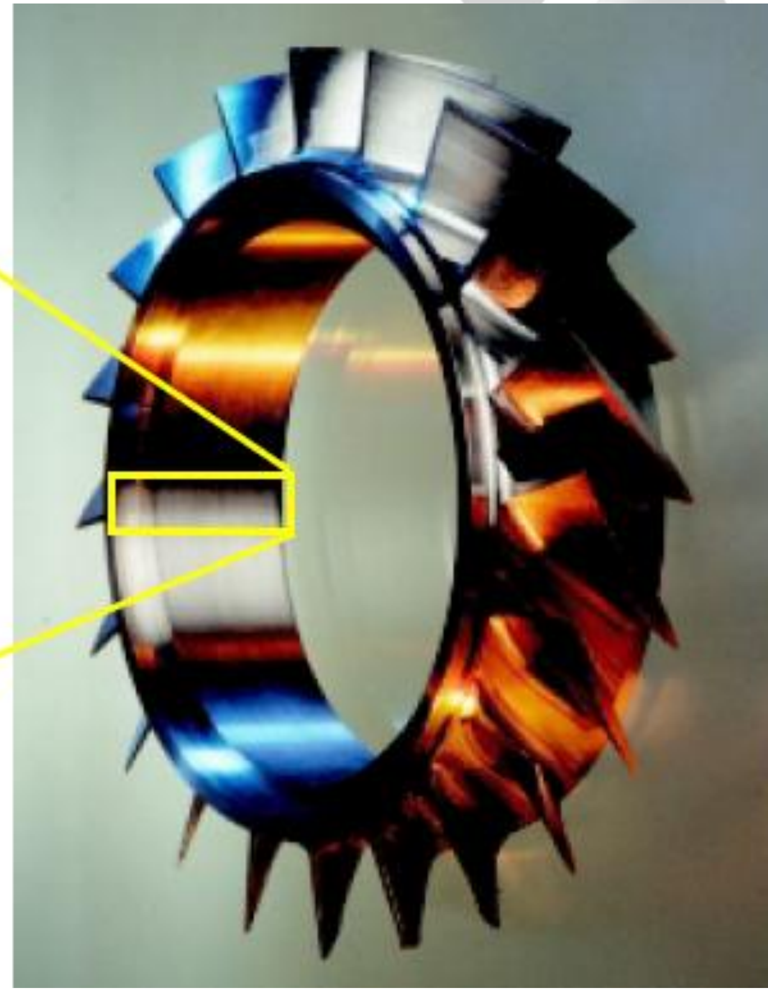
Source: Professor Neil Bourne

Correlating stress and damage

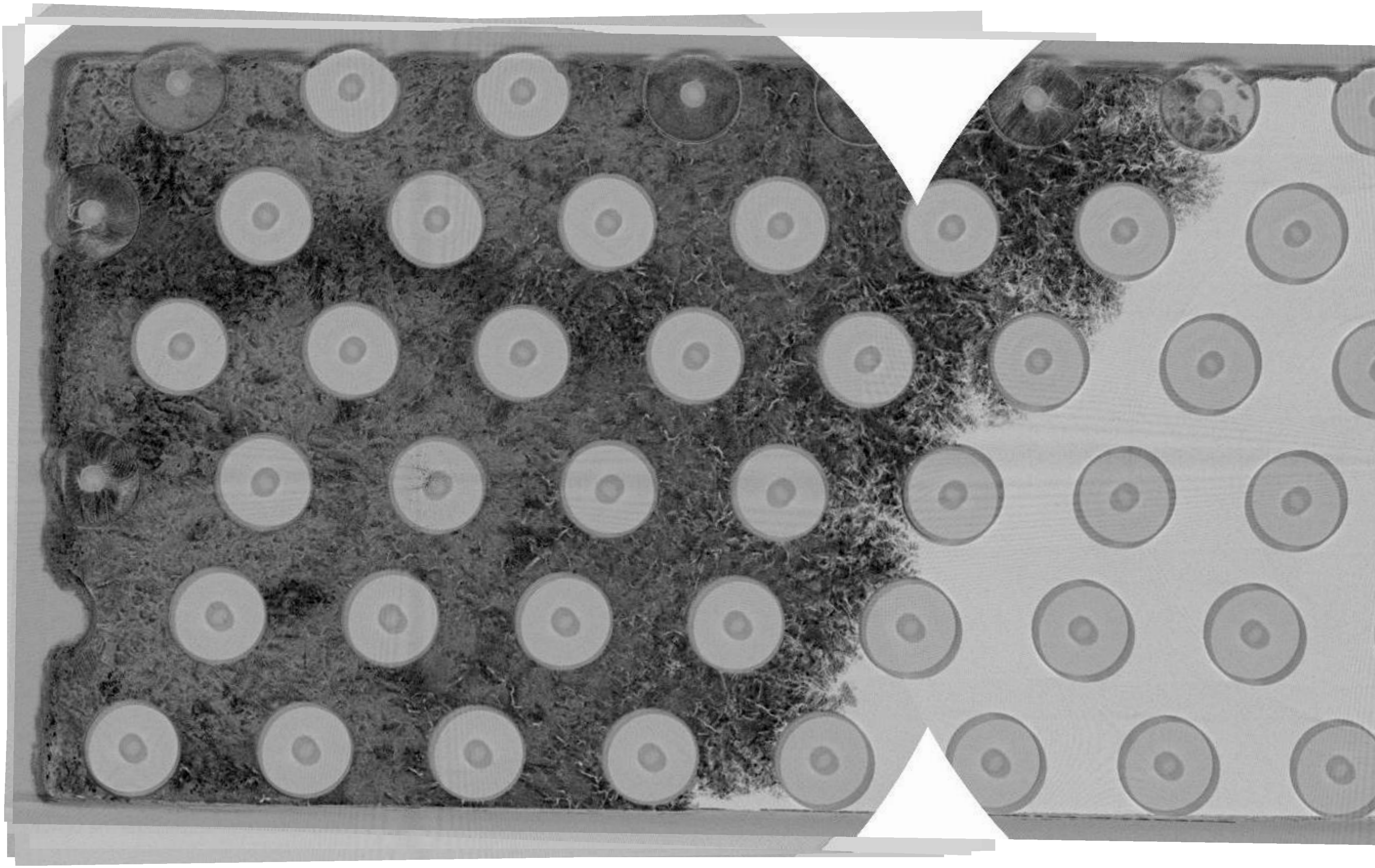
Ti/SiC metal matrix composites



Source: Professor Philip Withers

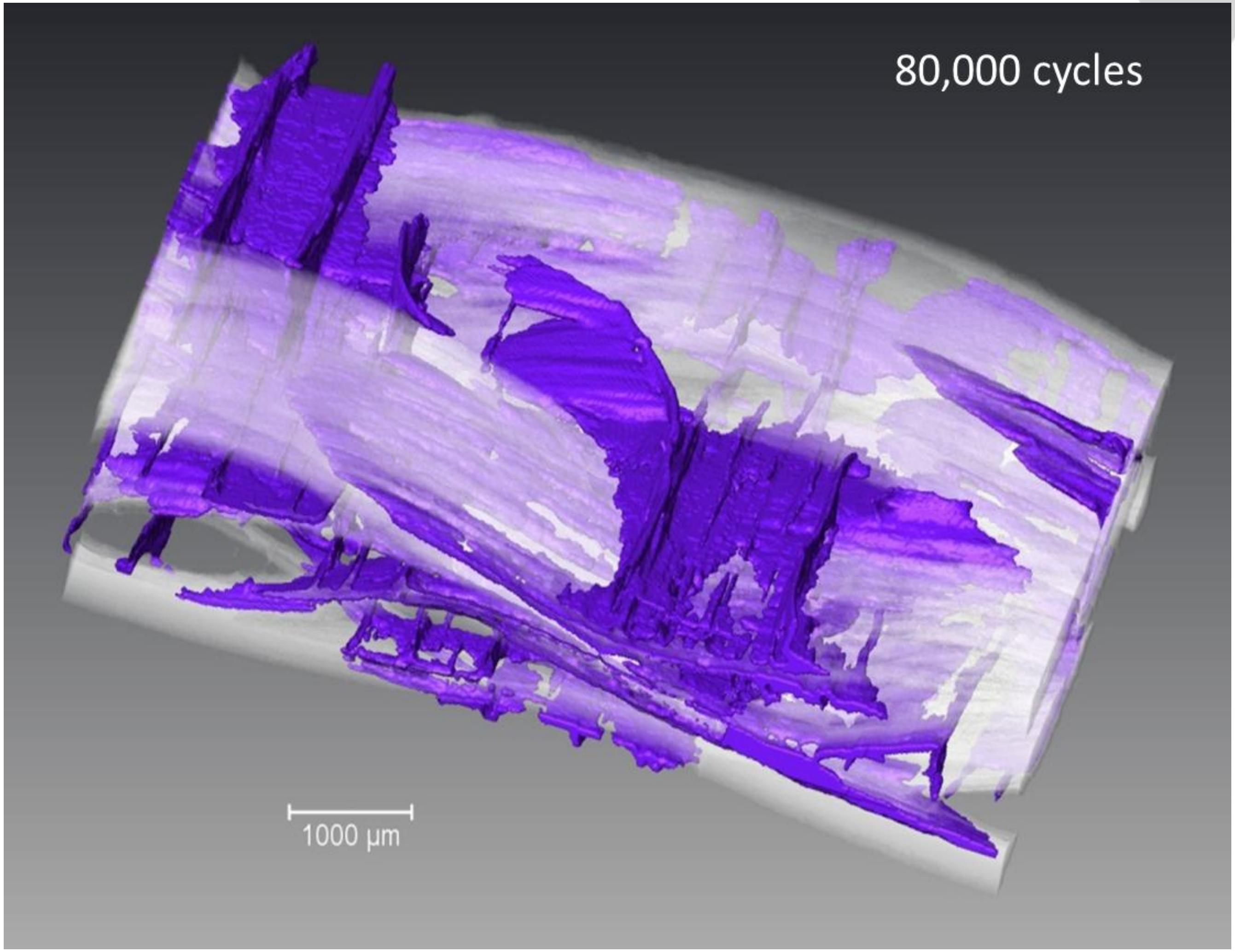


Fatigue crack growth over time



Source: Professor Philip Withers

Progressive damage over time



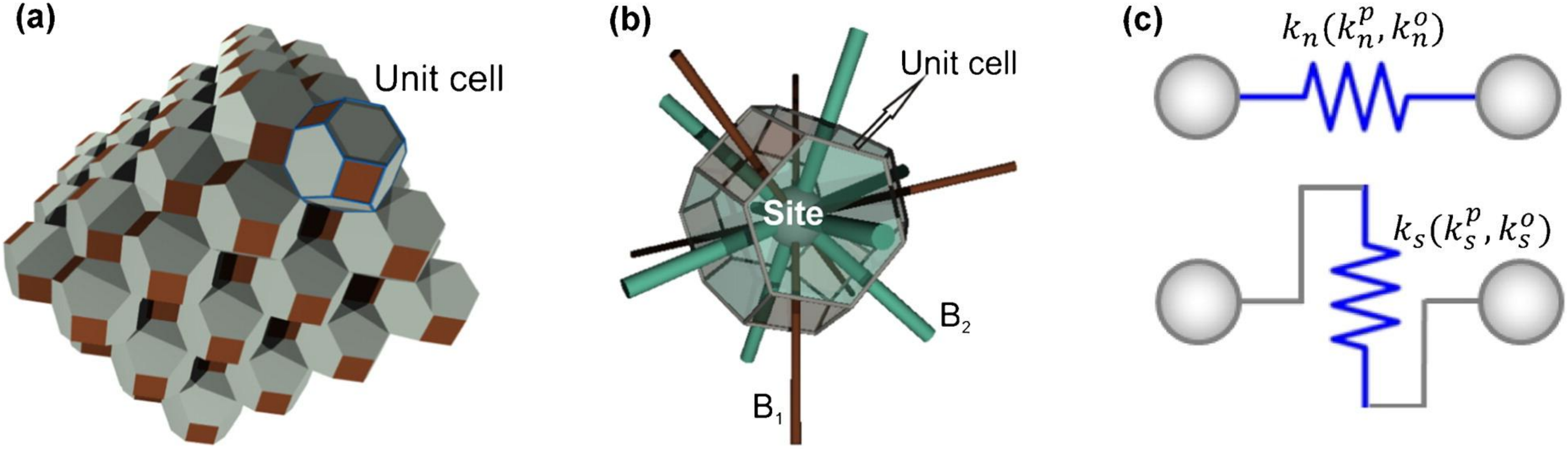
Source: Yu, Stein, Leonard, Withers, Soutis ECCM 14, 2014

Multiscale Modelling

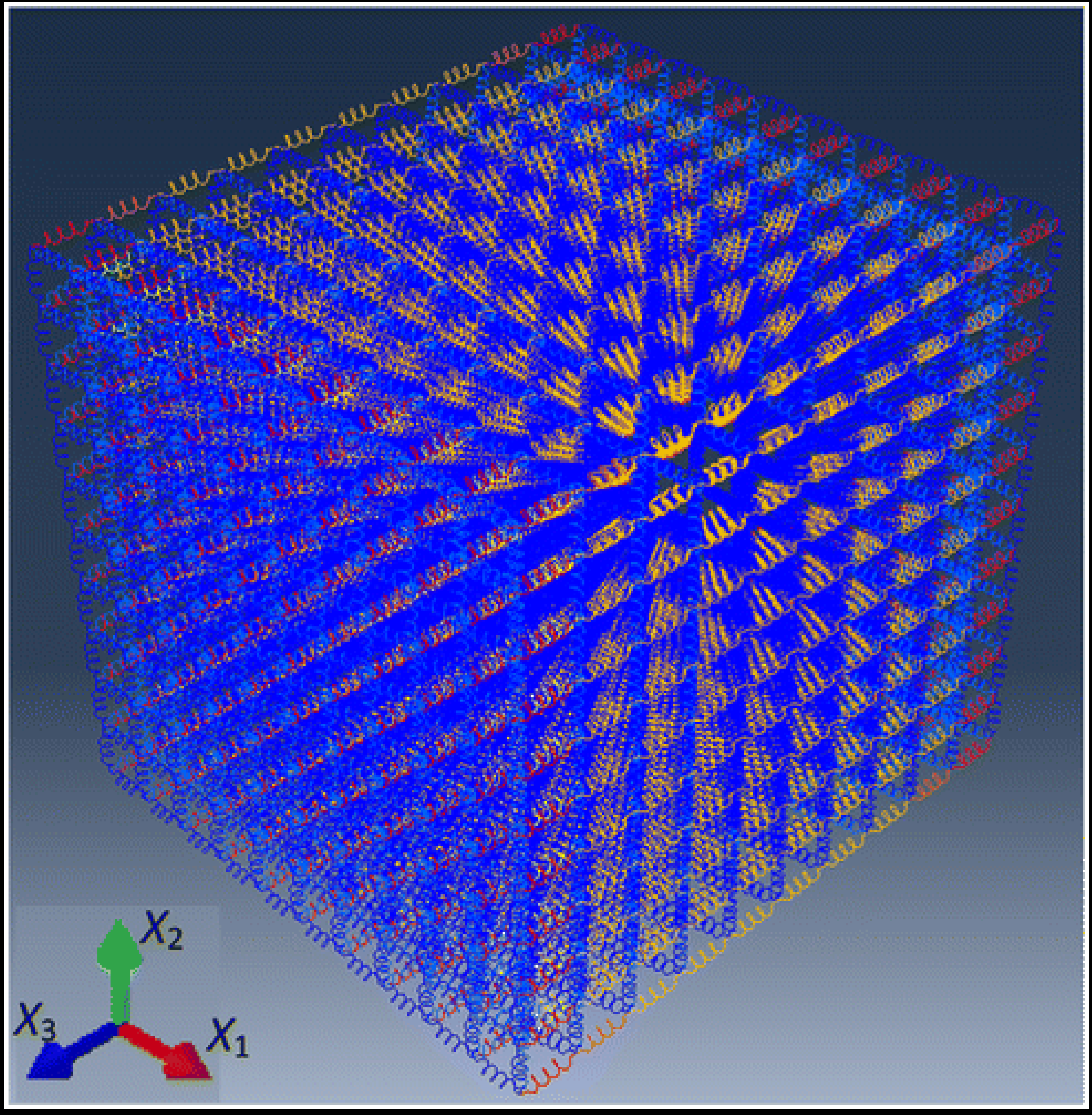
Meso-scale models

- Lattice-based or cellular automata ...
- Simulate mechanisms at grain scale
- Emergent behaviour such as fatigue/fracture
- Iterative 2-level process
  - Meso-scale updates FE scale continuum properties
  - FE computes new stresses

#1 Site-bond lattice models

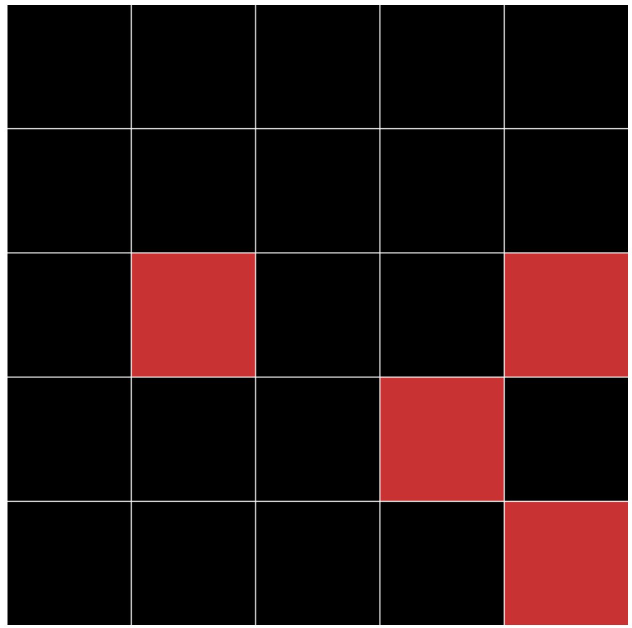


Zhang M. Morrison C.N. and Jivkov, (2014) Meso-scale site-bond model for elasticity: theory and calibration, Materials Research Innovations, Volume 18, Issue S2

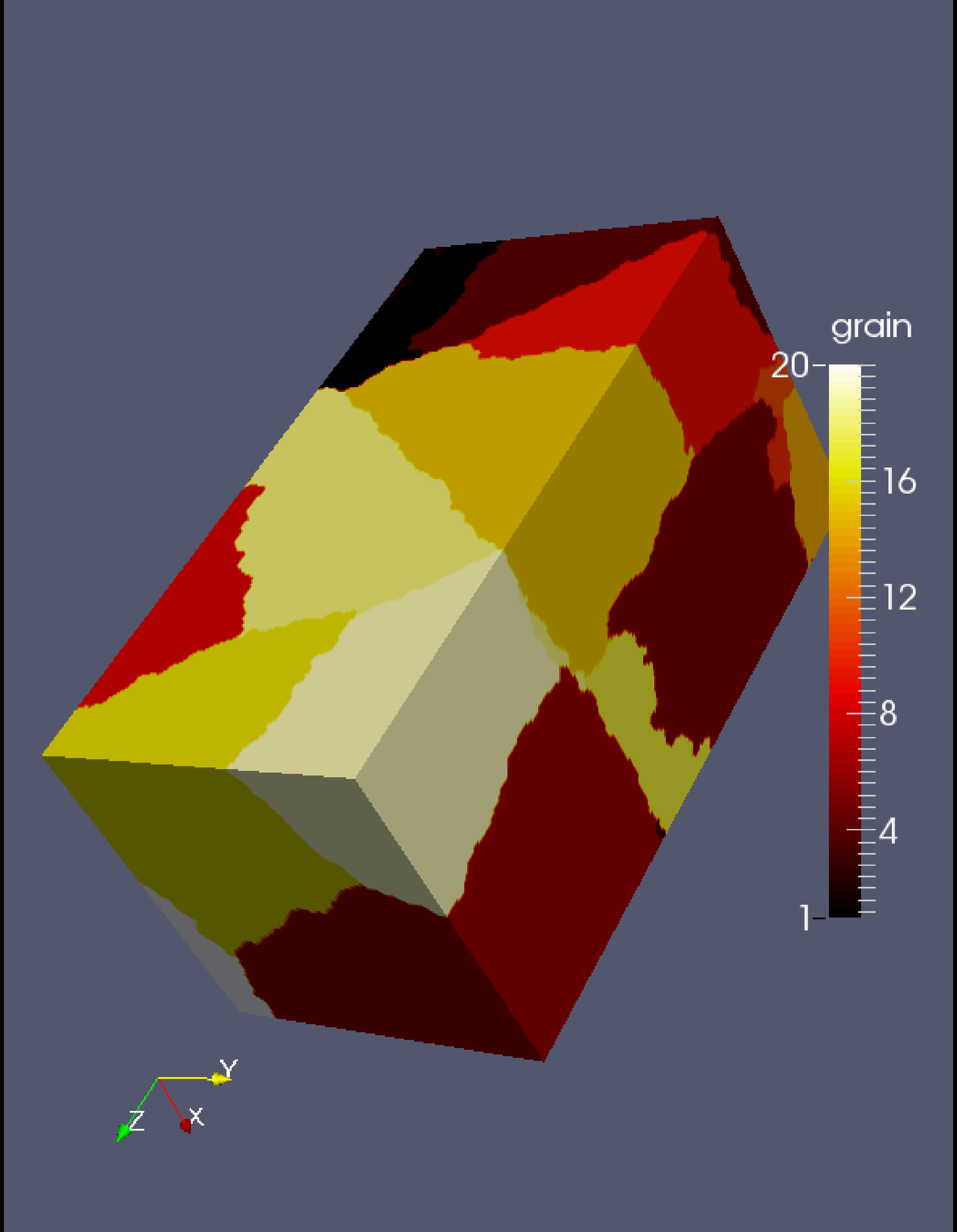


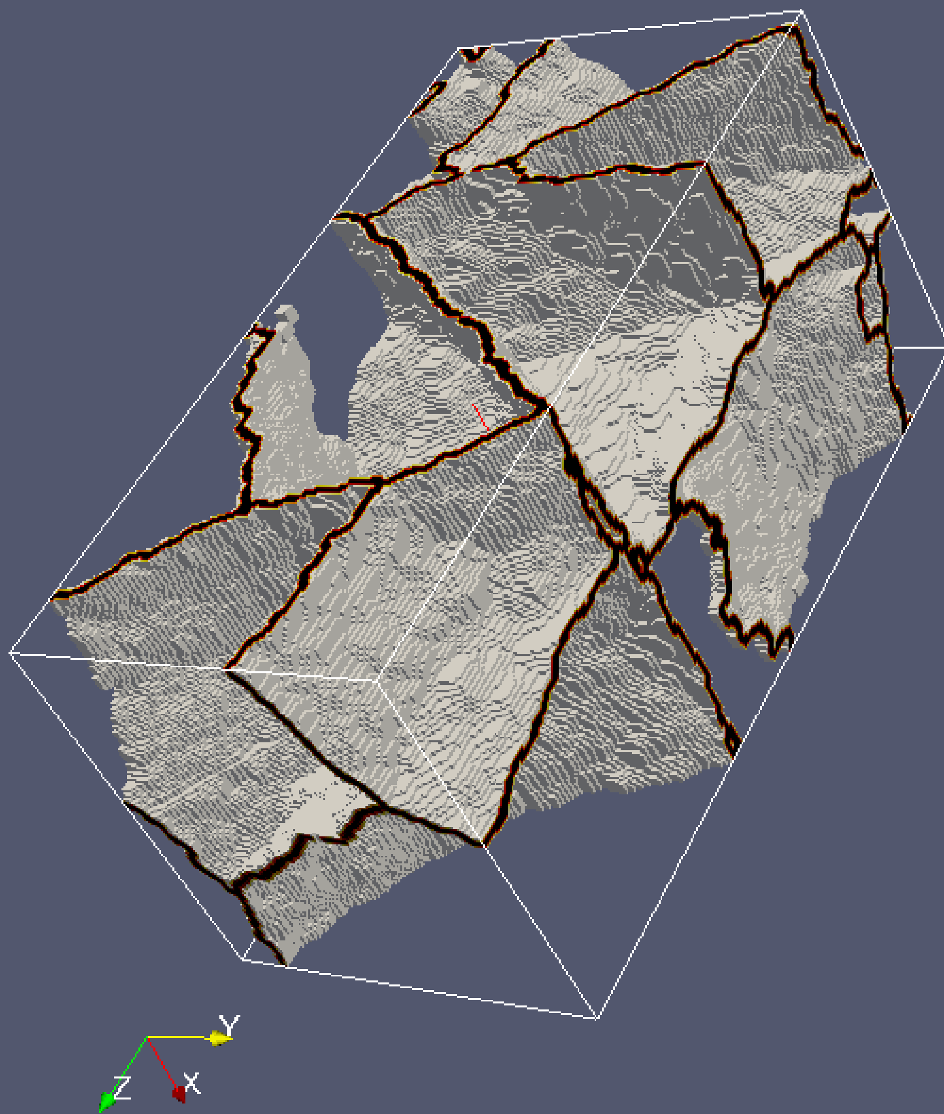
X_2
X_3
X_1

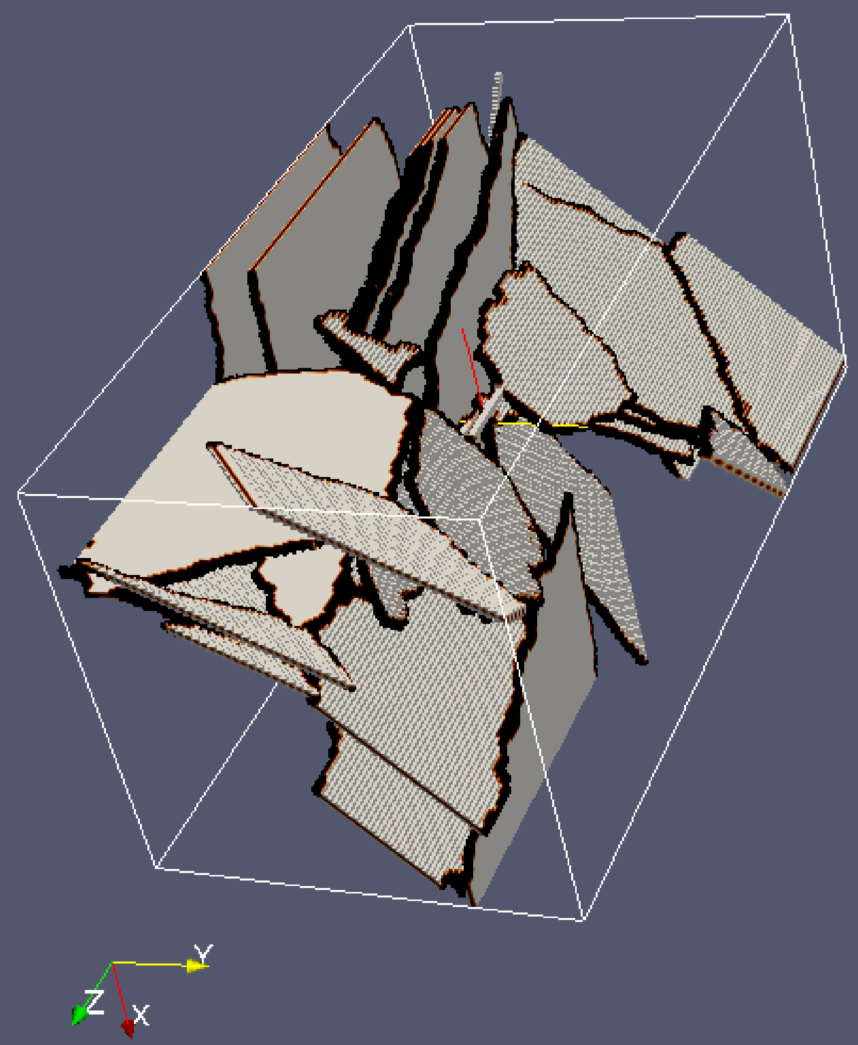
2# Cellular automata



Shterenlikht A. and Howard I.C. (2006) “The CAFE model of fracture – application to a TMCR steel”, Fatigue and Fracture of Engineering Materials and Structures, Volume 29, Issue 9-10


grain
20
16
12
8
4
1
Y
Z
X


Y
Z
X


Y
Z
X

Summary

Fatigue modelling in the future

- May involve a two-level strategy based on modelling mechanisms in the meso-scale
- Research activity over next 5 years enabled by HPC facilities and OSS
- Verification and validation of the methodology using 4D tomography
- Use in industry in next 5-10 years through desktop ISV packages

Acknowledgements

- N8 HPC Access to Polaris
- PRACE DECI-10 Access to Mare Nostrum
- EPSRC Access to HECToR
- PRACE DECI-12 Access to Blue Joule
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- UK Software Sustainability Institute