Visual Analytics, HPC, Simulations & AI

Tomasz Bednarz (CSIRO Data61, UNSW)

and

John Taylor (CSIRO Data61, DST)

About Tomasz

- **Director of Visualisation** at the Expanded Perception and Interaction Cente, UNSW Art & Design
- **Team Leader** (Visual Analytics) at the CSIRO/Data61
- **Adjunct Associate Professor** at the Queensland University of Technology, Applied and Computational Mathematics (ACM)
- **Adjunct Associate Professor** at the University of Sydney, Design Lab
- **Adjunct Senior Lecturer** at the University of South Australia, School of Information Technology and Mathematical Sciences
- **Courses Chair** at the SIGGRAPH Asia 2017
- **Chair** at the SIGGRAPH Asia 2019

About John

- **Group Leader** (Computational Platforms) at the CSIRO/Data61
- **Program Leader,** HPC and Computational Science at the Defence Science and Technology
- **Adjunct Professor**, School of Computer Science, Australian National University

DATA 61

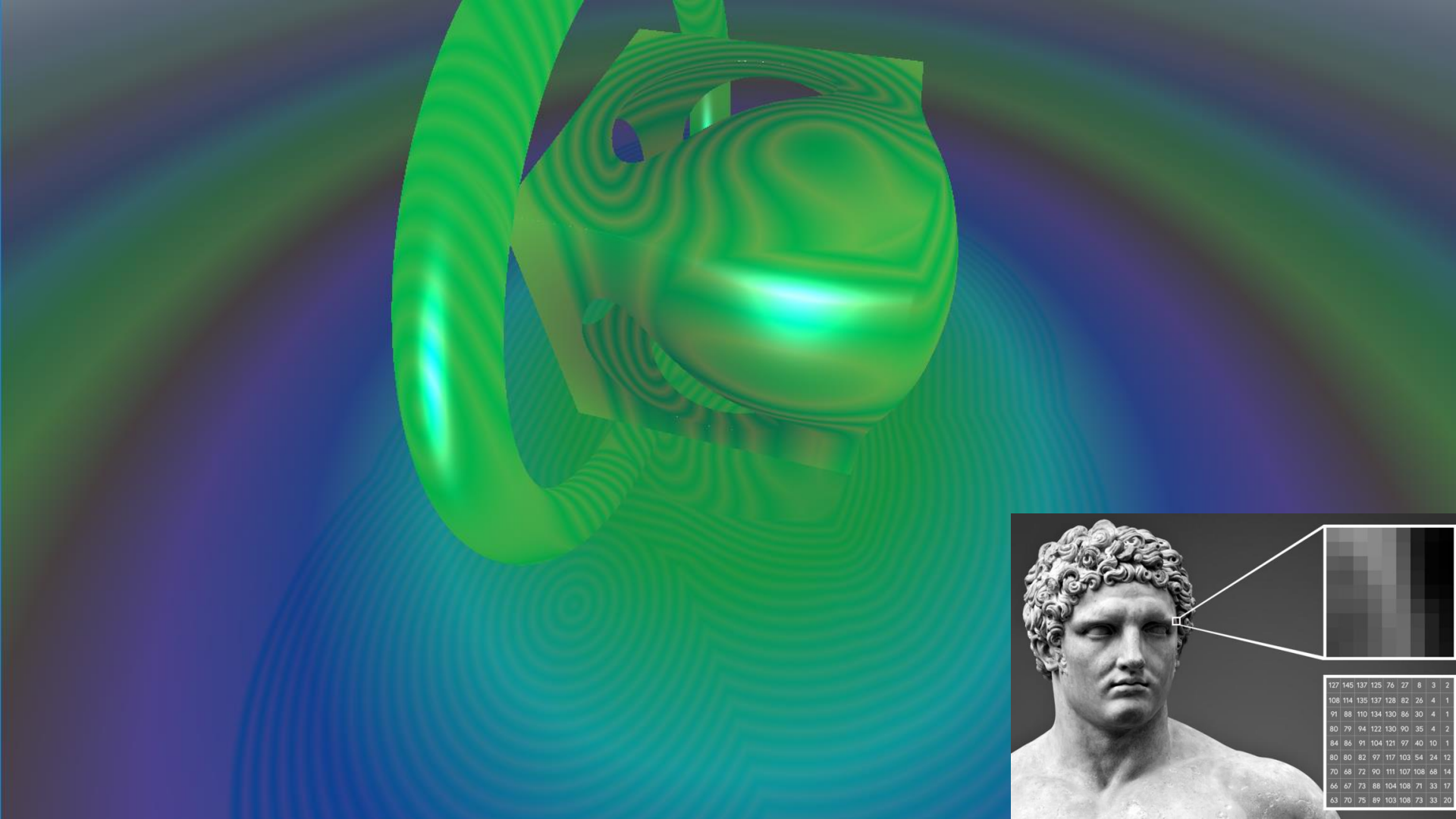
CSIRO

Australian National University

Australian Government

Department of Defence

Science and Technology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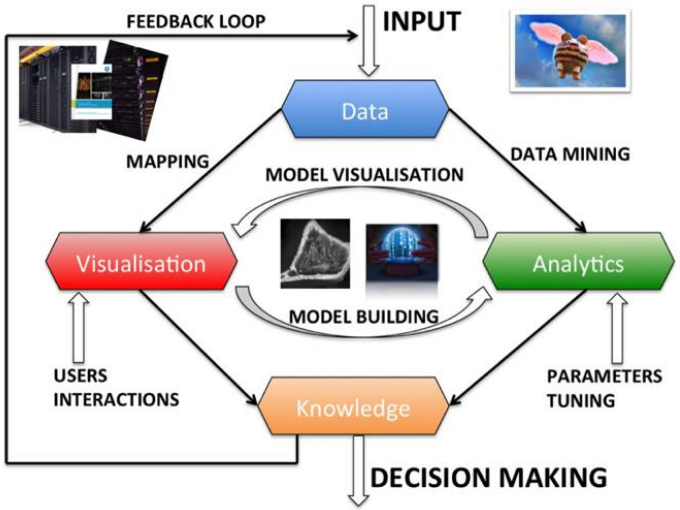
70 68 72 90 111 107 108 68 14
66 67 73 88 104 108 71 33 17
63 70 75 89 103 108 73 33 20

Role of Visualisation

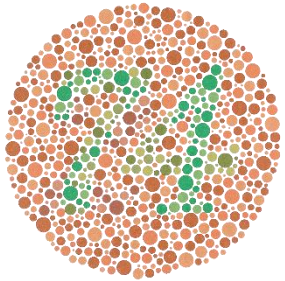
- **Human in the loop**
- Display information
  - photographs, plots, trends.
- Analyse data to support reasoning
  - develop and assess hypotheses
  - discover errors in data
  - expand memory
  - find patterns
  - make decisions.
- Communicate
  - share and persuade
  - collaborate and revise.

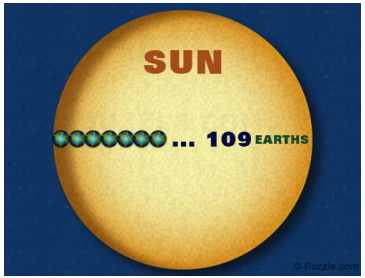


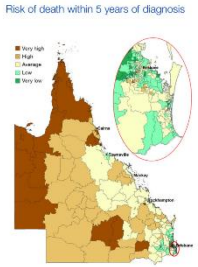
Effective Visual Communication

- Colour (highlight important information)
- Typography (fonts for communication style)
- Layout (logical hierarchy, consistency)
- Callouts (highlight key information)
- Space (avoid clutter and incoherence)

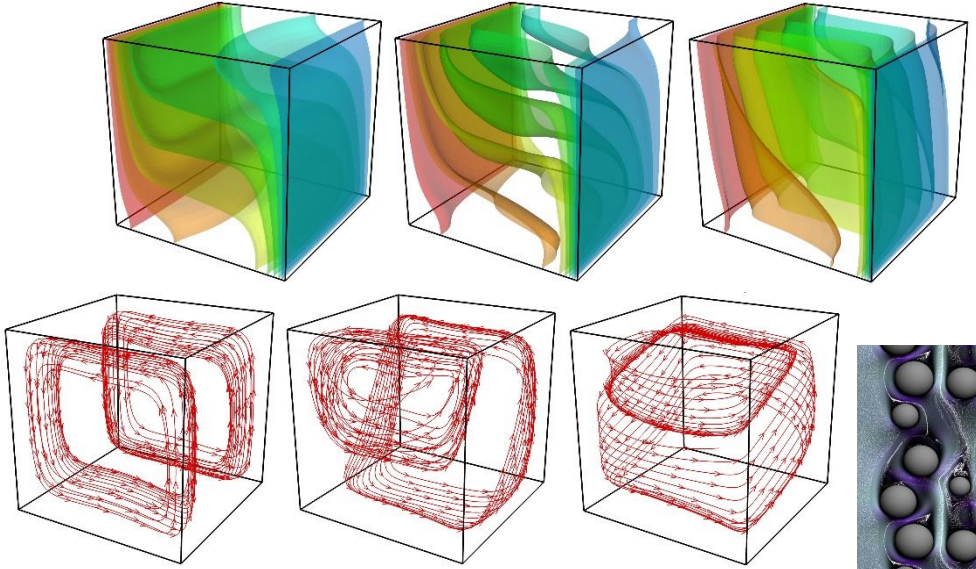
- Illustration (to enhance the content)
- Iconography (enhance comprehension)
- Data (reveal patters using visuals)
- Proportion (items properly sized)
- Simplicity (zen of visualisation)

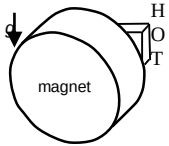


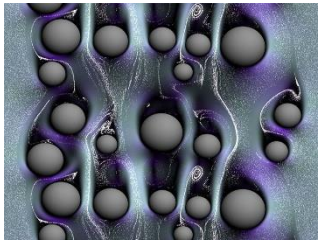


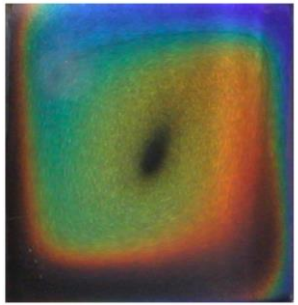


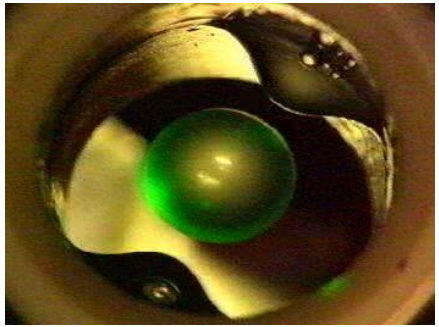
Physics and Vis



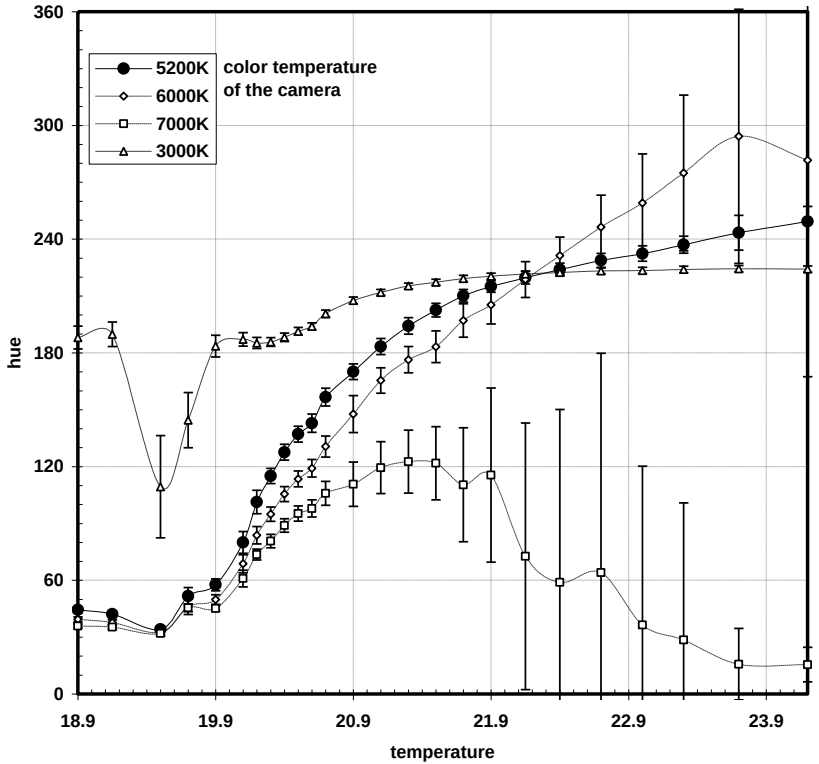


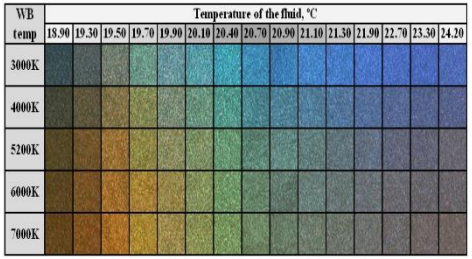


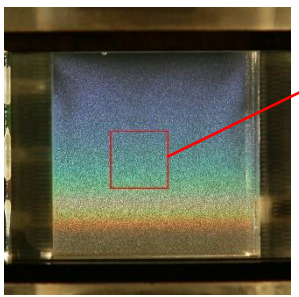


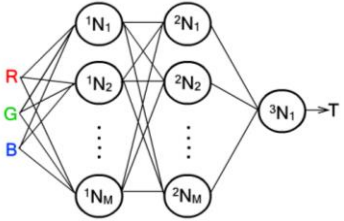


From Visualisation to Measurement using AI









No.	Input parameters	Neurons in layers	Activation functions	Color bandwidth [ºC]	Regression coefficient	Mean absolute error [ºC]
1	H	polynomial fit		19.7 – 23.7	0.9962	0.0493
4	R, G, B	6, 6, 1	log, log, lin	19.7 – 23.7	0.9898	0.0733
11	R, G, B, H	20, 20, 1	log, log, log	19.7 – 23.7	0.9978	0.0319
12	R, G, B	3, 3, 1	log, log, log	18.9 – 24.2	0.9810	0.1129

CSIRO
Bracewell GPU Cluster

CSIRO Bracewell GPU Cluster

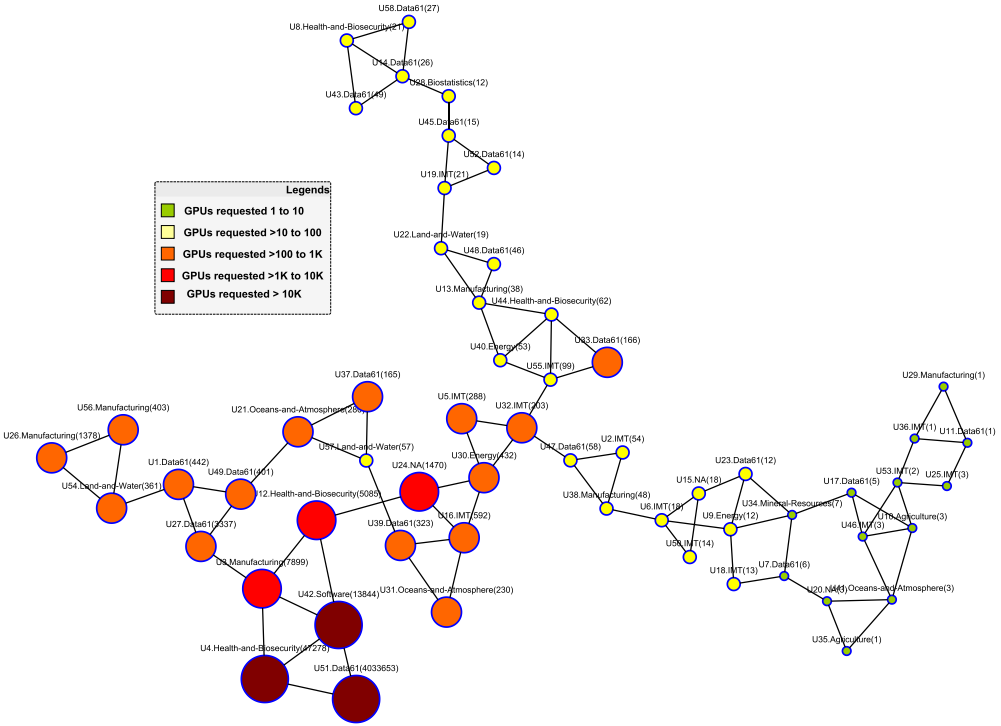
The most powerful supercomputer in Australia

- Bracewell consists of 114 PowerEdge C4130 servers hooked together with EDR InfiniBand.
- Aggregate memory across the entire system is 29 TB.
- Each server is equipped with four NVIDA P100 GPUs and two Intel Xeon 14-core CPUs.
- The GPUs alone represent over 2.4 petaflops of peak performance.
- Bracewell was installed over a period of just five days spanning the end of May and beginning of June 2017.
- The system came online in early July 2017

CSIRO Bracewell GPU Cluster

Bragg Cluser Usage

- During 27 April – 27 May
  - 50 users running GPU jobs
  - 30,348 GPU jobs run
    - Computational modelling
    - Image processing
    - Virtual nanoscience
    - Molecular modelling
    - Environmental modelling
    - Physiological modelling
    - Bioinformatics
    - Machine learning

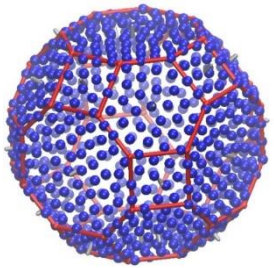


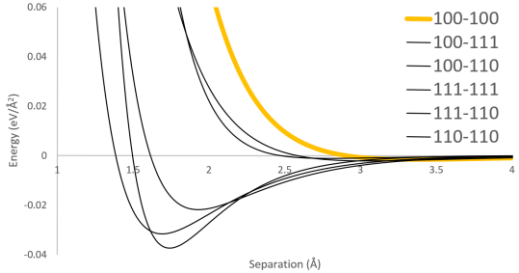
Source: CSIRO IMT Ahmed Arefin & Steve McMahon

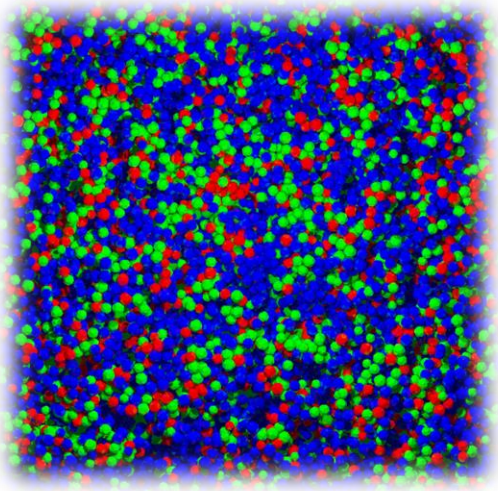
SNAP – Simulated Nanostructure Assembly using Proto-particles

Allows creation of user-defined nanoparticles, and subsequent Molecular Dynamics simulation to study aggregation.

Nanoparticles are represented using a surface mesh, enabling researchers to define complex combinations of sizes, shape and facet combinations, each with specifically defined interactions.







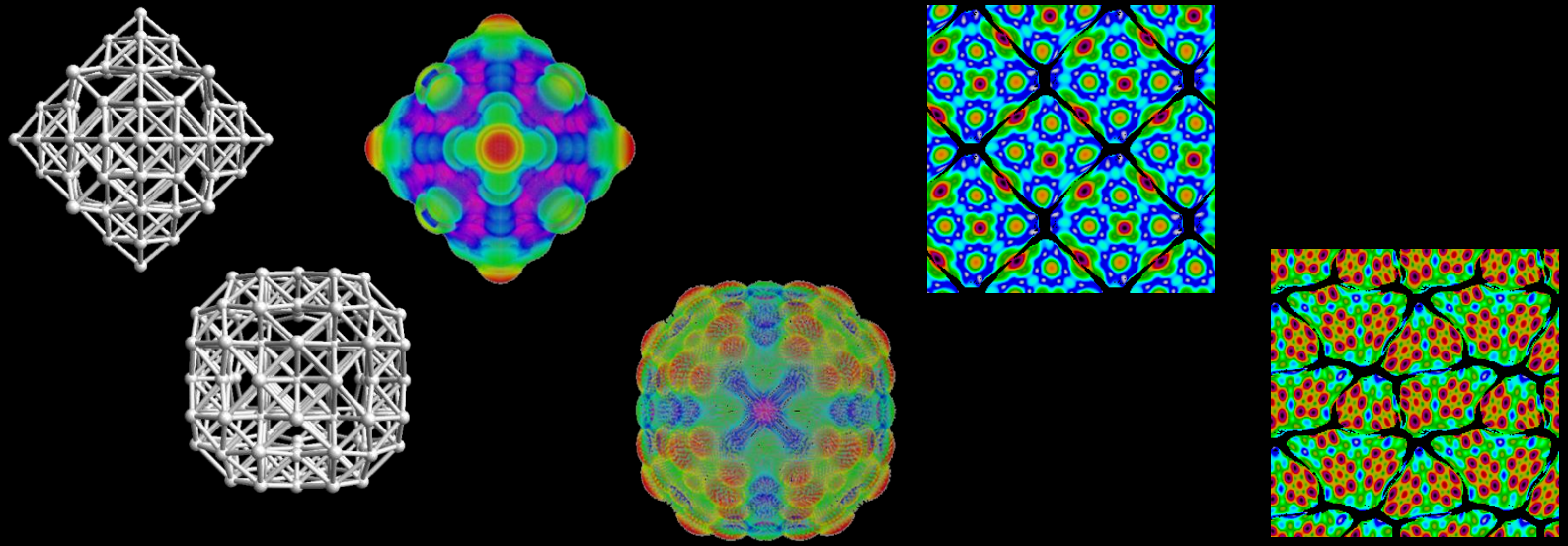
GPU enabled to allow scaling to > 50,000 complex zonohedrons.

Includes tools for generating nanoparticle surface meshes and post simulation analysis.

https://research.csiro.au/mmm/snap/

Materials Informatics & Data-driven Discovery

- Analysis of High-Throughput Computation
- Data representation, Machine- and Deep-Learning approaches



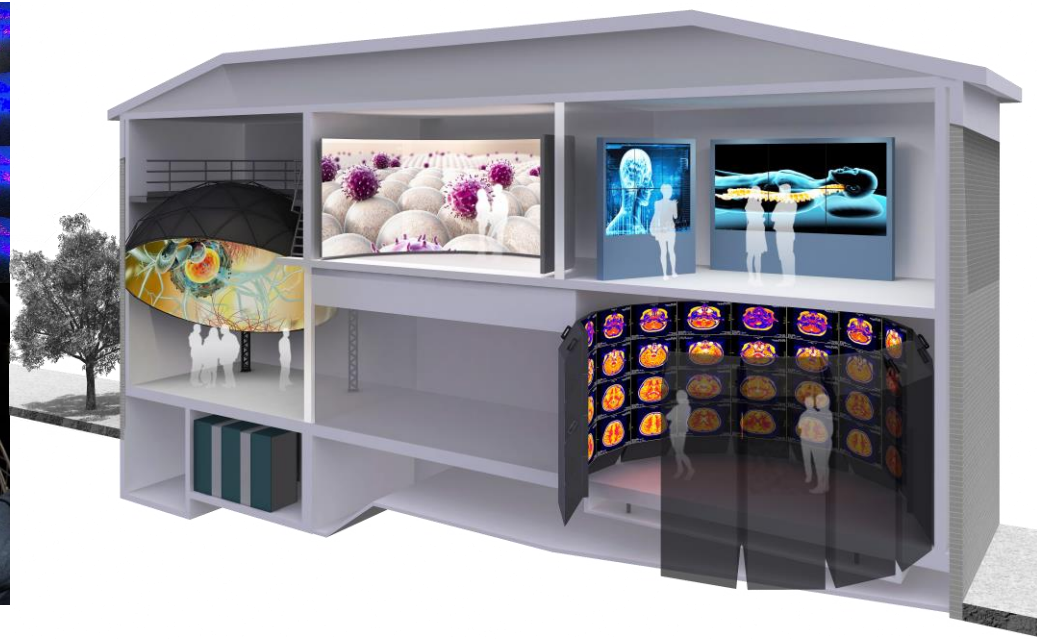
Defence Science and Technology

- Developing HPC capability to support defence research
- Pilot system has been acquired that includes V100 GPUs
- Strong interest in application of AI and deep learning to Defence
- Full system will be in the top 50 of the TOP500 supercomputers
- Legacy codes including commercial applications, eg CFD applications will need significant work to run efficiently on GPUs.

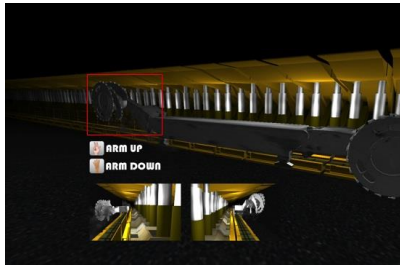
Expanded Perception & Interaction Centre

EPICentre

- EPICylinder
- DomeLab
- XR-LAB
- Avie-SC

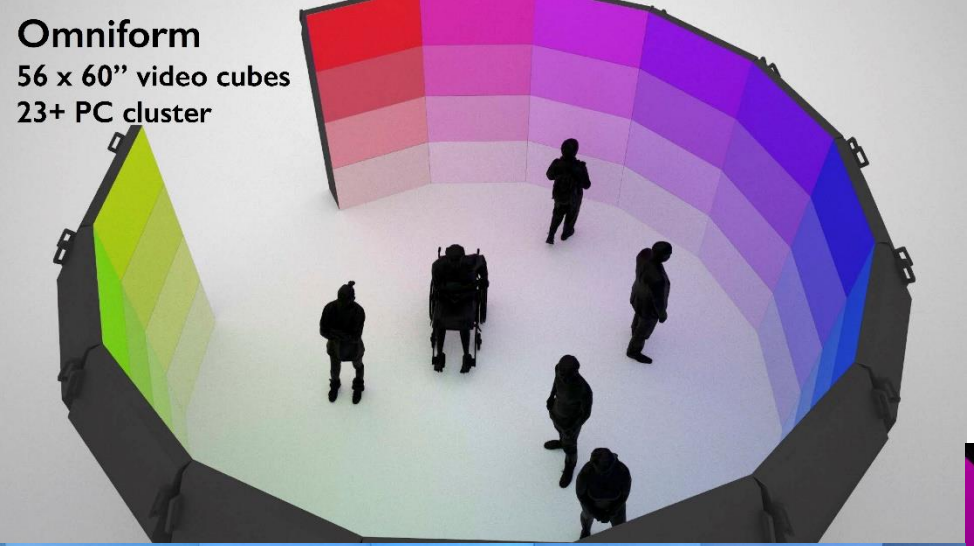


Milgram’s Reality Virtuality Continuum



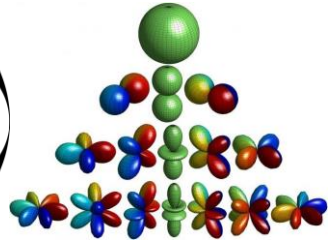
The area between the completely real and completely virtual, consists of both augmented reality, where the virtual augments the real, and augmented virtuality, where the real augmented the virtual.

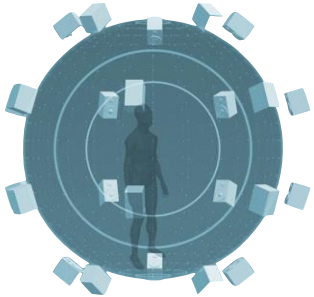
P. Milgram and A.F. Kishino, Taxonomy of Mixed Reality Visual Displays, IEICE Transactions on Information and Systems, E77-D(12), pp. 1321-1329, 1994.



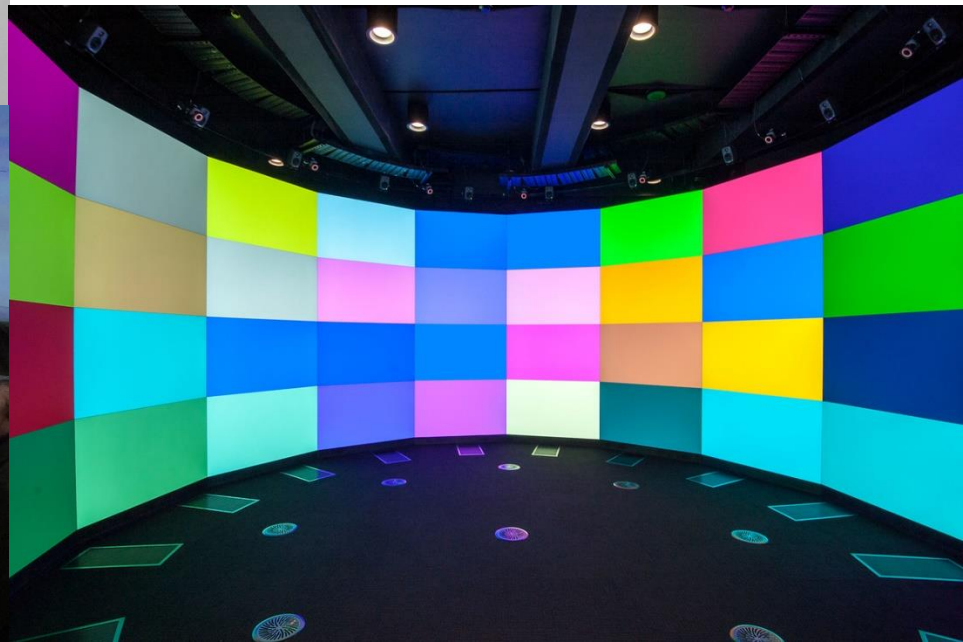
Ambisonics
32+1 speaker array

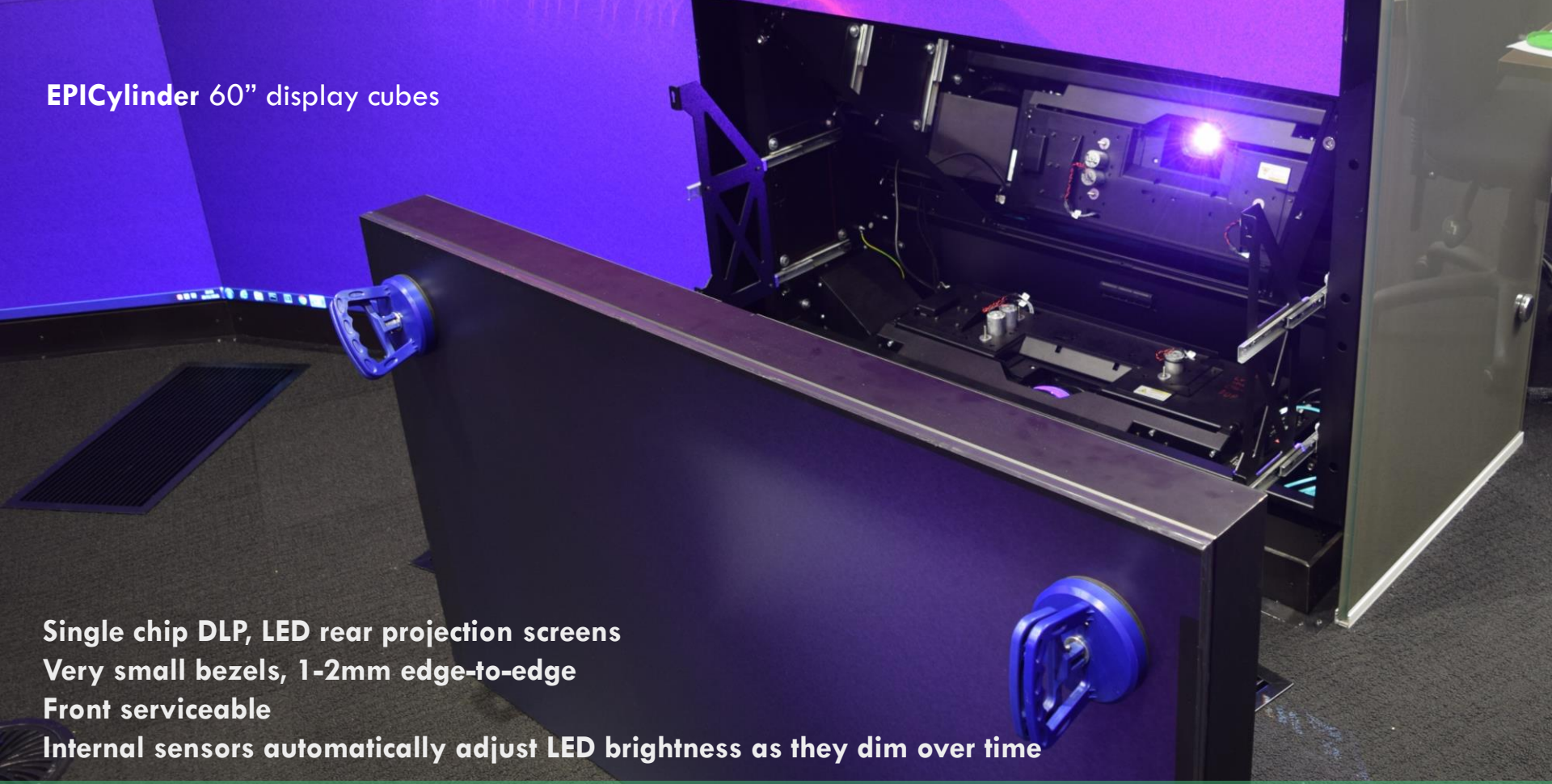
EPICentre





Immersive and Big Data Visualisation



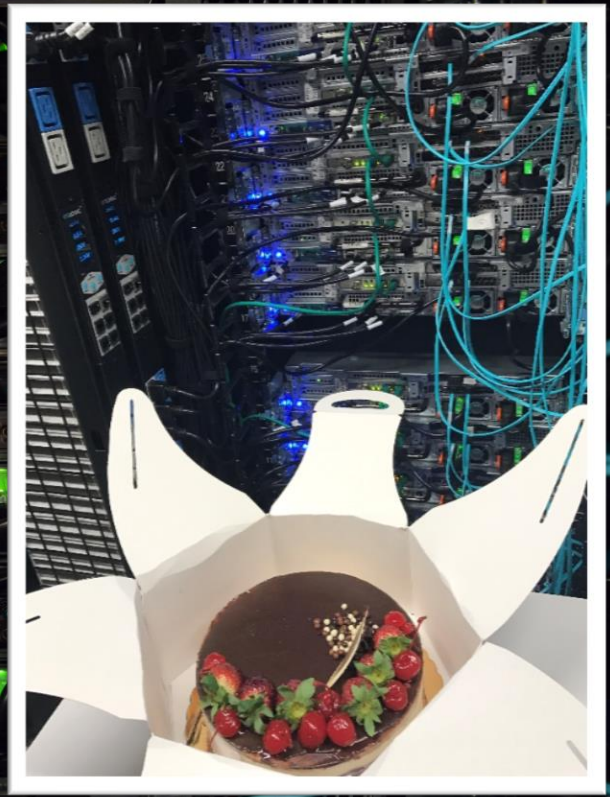


EPICylinder 60” display cubes

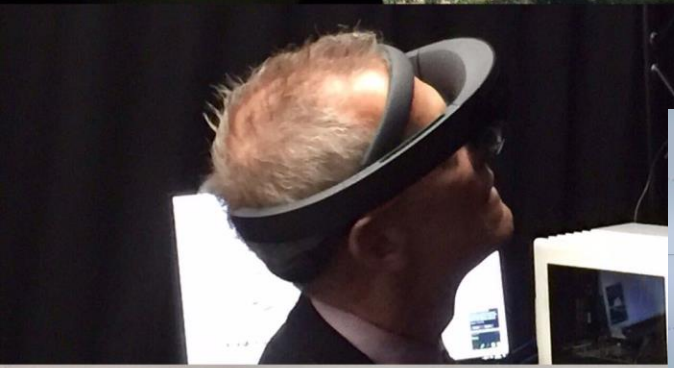
Single chip DLP, LED rear projection screens
Very small bezels, 1-2mm edge-to-edge
Front serviceable
Internal sensors automatically adjust LED brightness as they dim over time

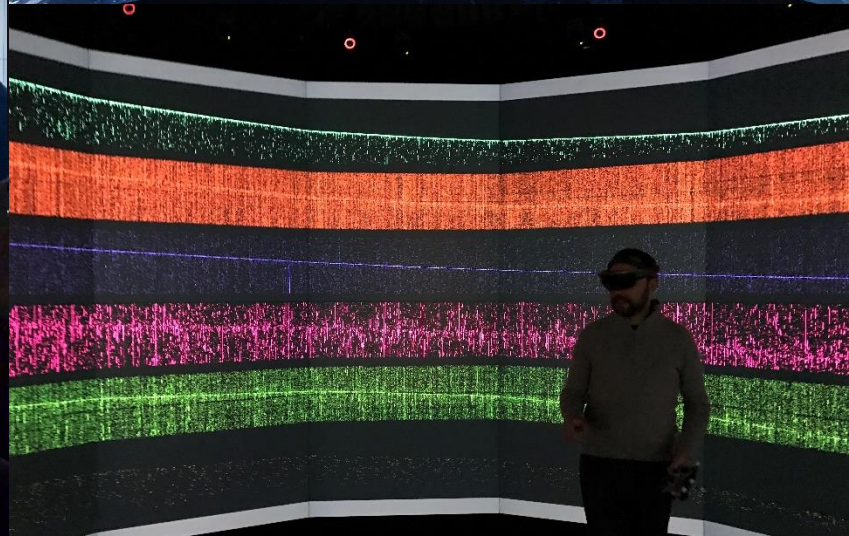
Server Room

28+1 cluster Xeon E5-2650 v3
nvidia quadro M6000 graphics cards with quadro sync
dual bonded 10Gbit/s ethernet
~3km of display port over fibre cable
16 node HPC cluster
200Tb file server

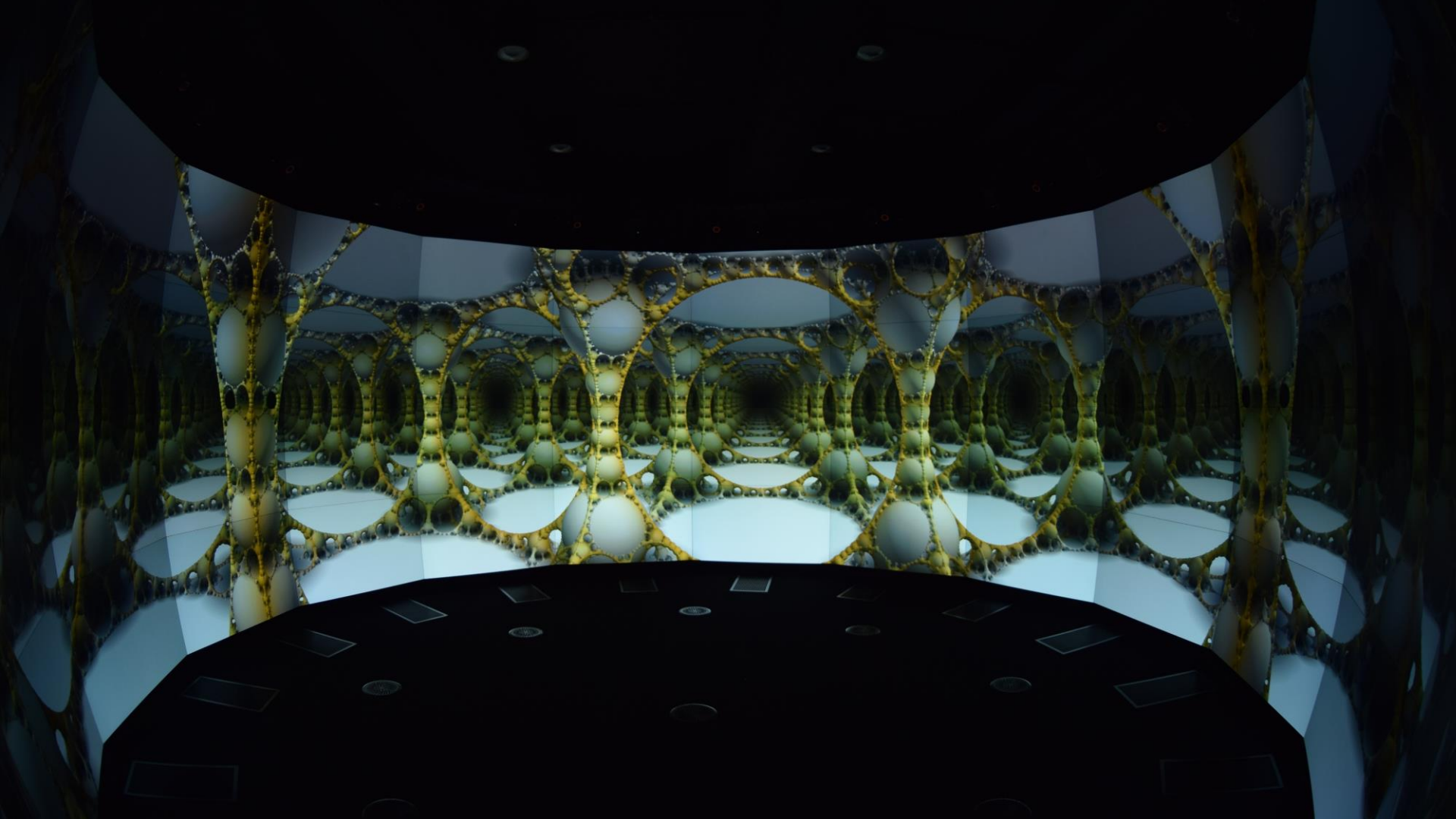


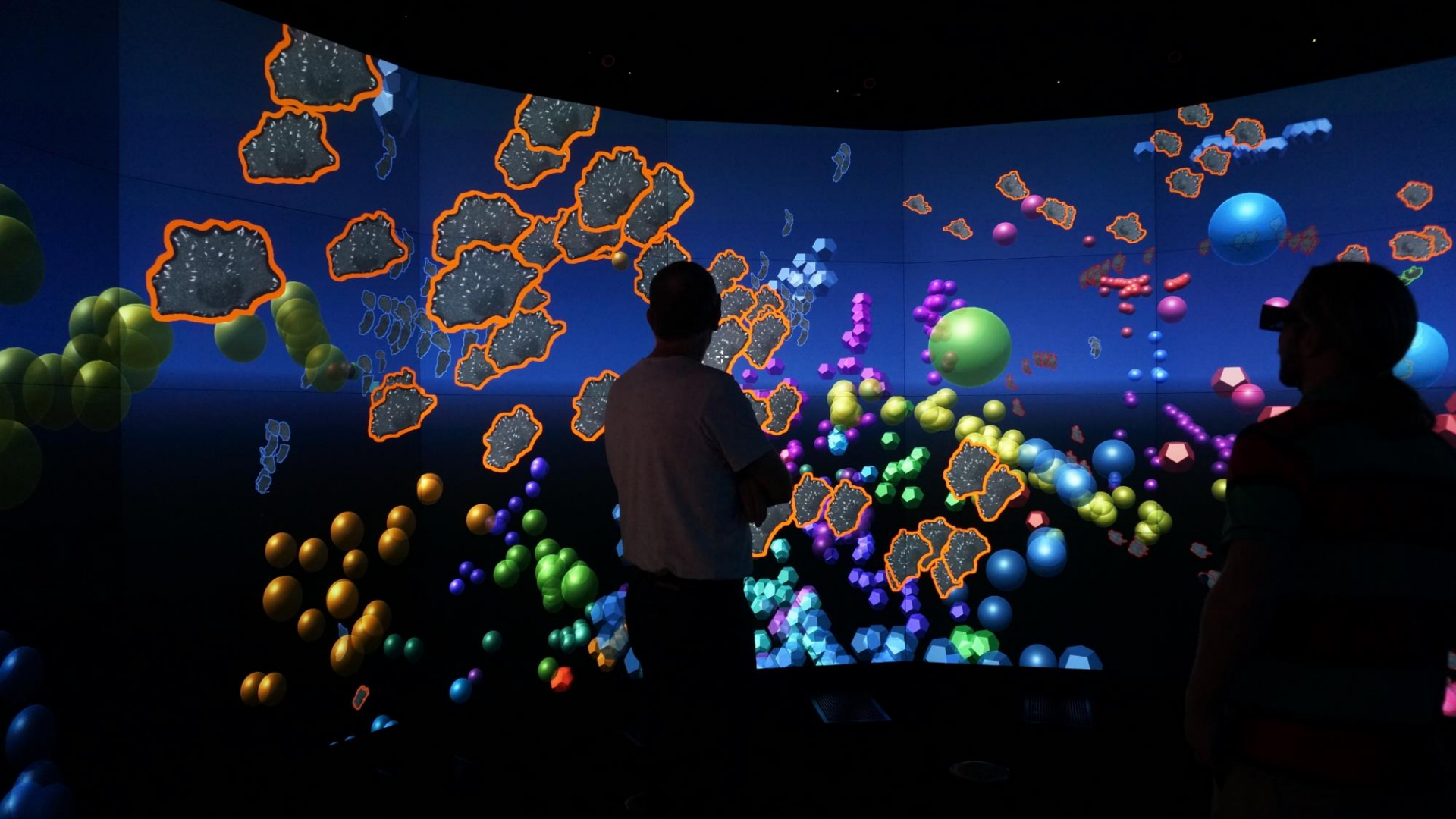
Xeon Processor E5-2650 v3



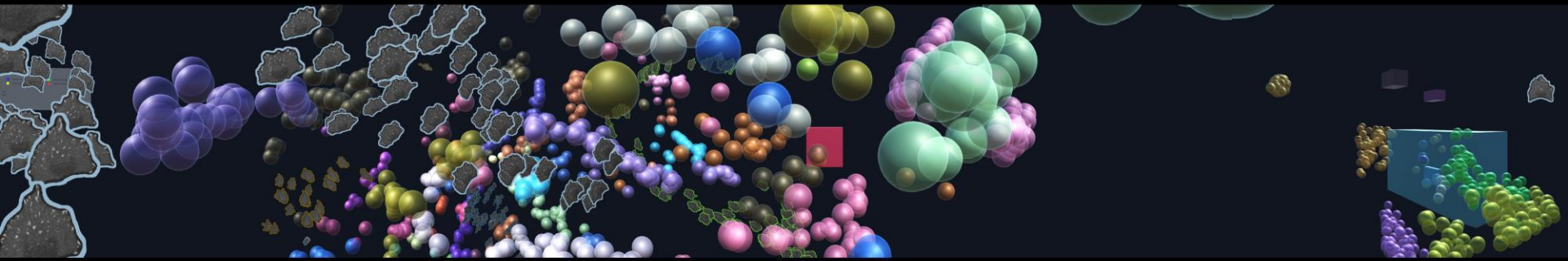


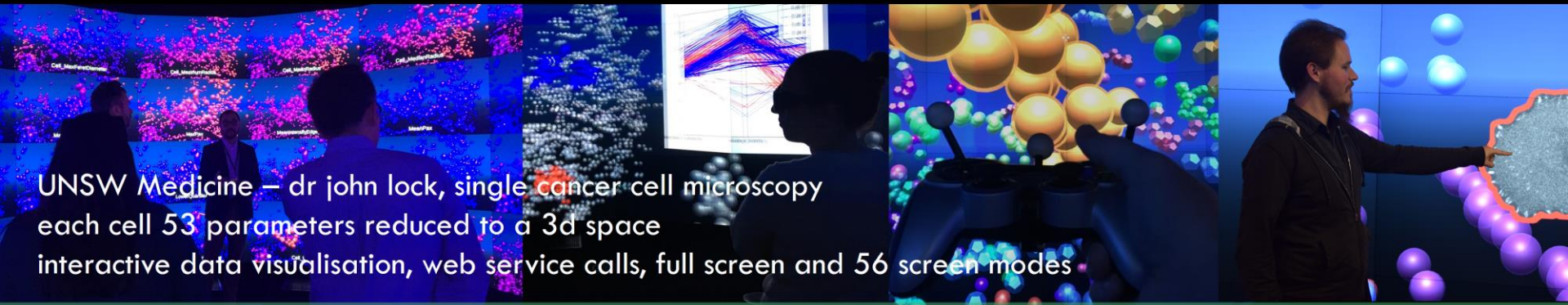
Immersive and Big Data Visualisation





single molecule science - interactive cancer cell visualisation in EPICylinder



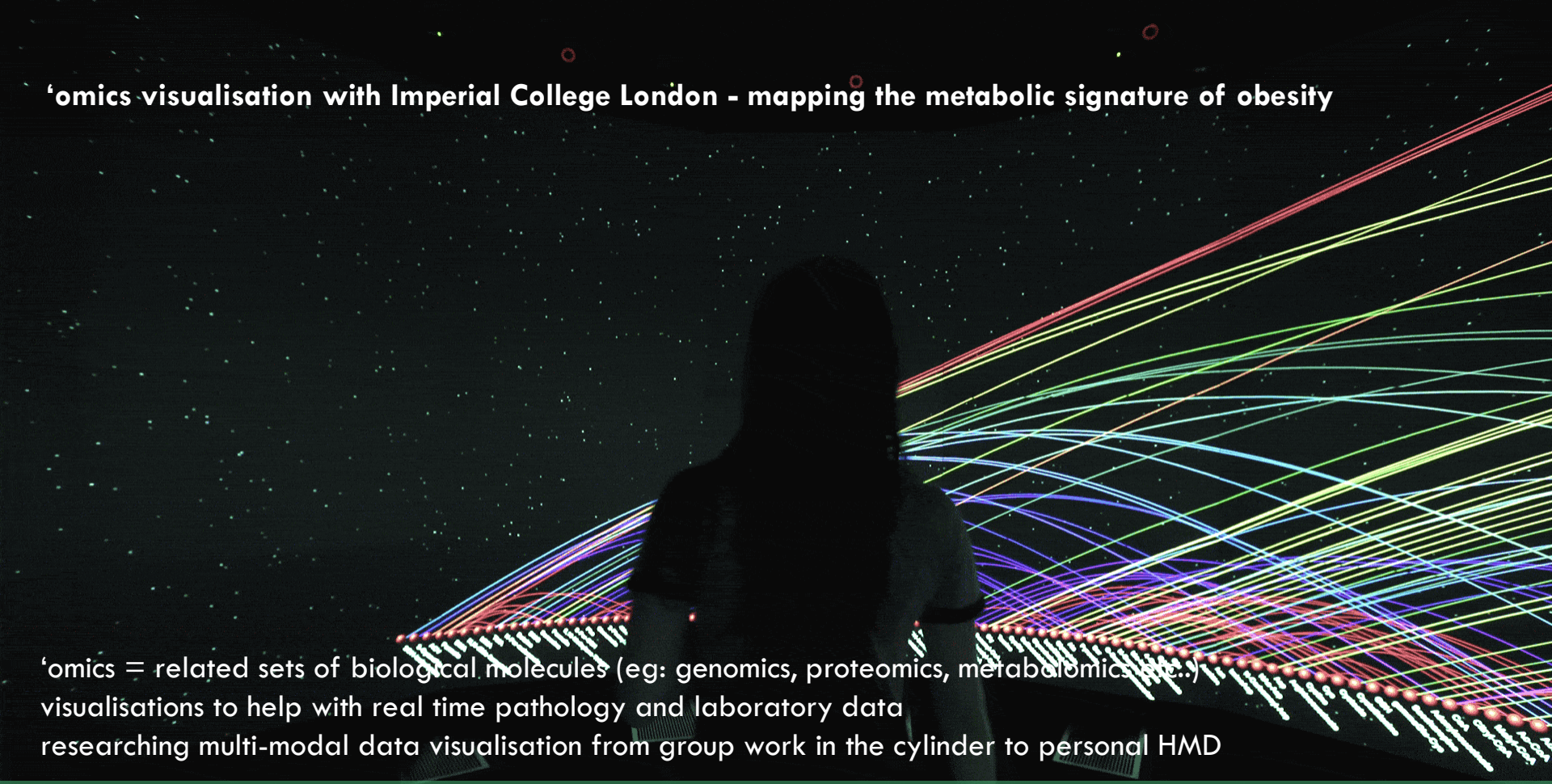


UNSW Medicine – dr john lock, single cancer cell microscopy
each cell 53 parameters reduced to a 3d space
interactive data visualisation, web service calls, full screen and 56 screen modes

EPICylinder Project

EPICentre

‘omics visualisation with Imperial College London - mapping the metabolic signature of obesity

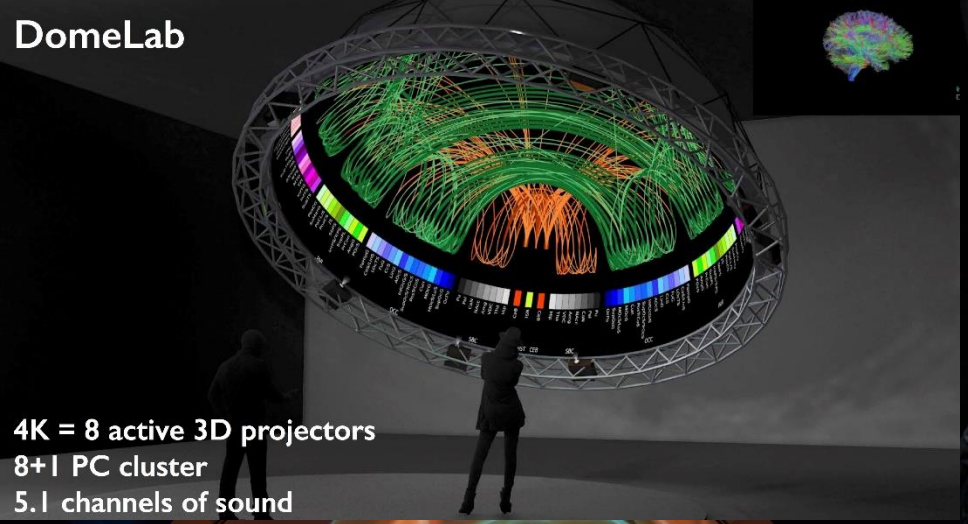


‘omics = related sets of biological molecules (eg: genomics, proteomics, metabolomics etc..)
visualisations to help with real time pathology and laboratory data
researching multi-modal data visualisation from group work in the cylinder to personal HMD

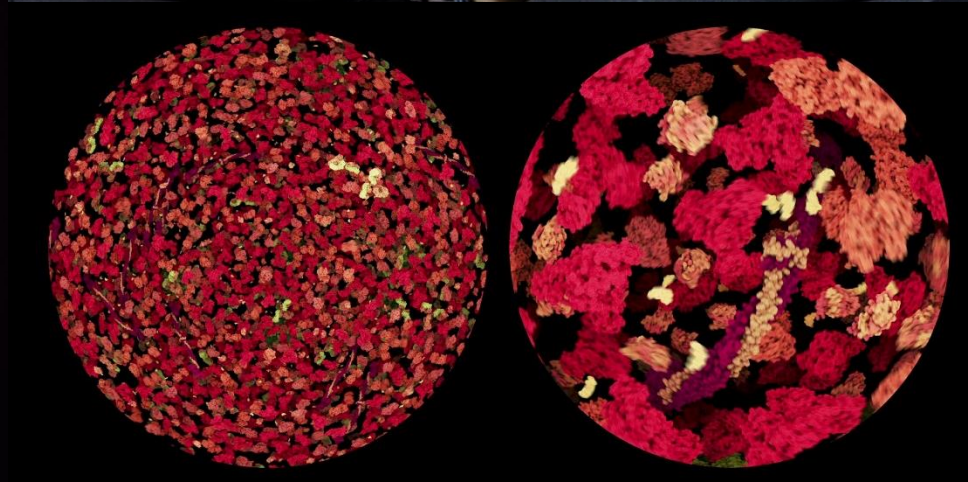
DomeLab

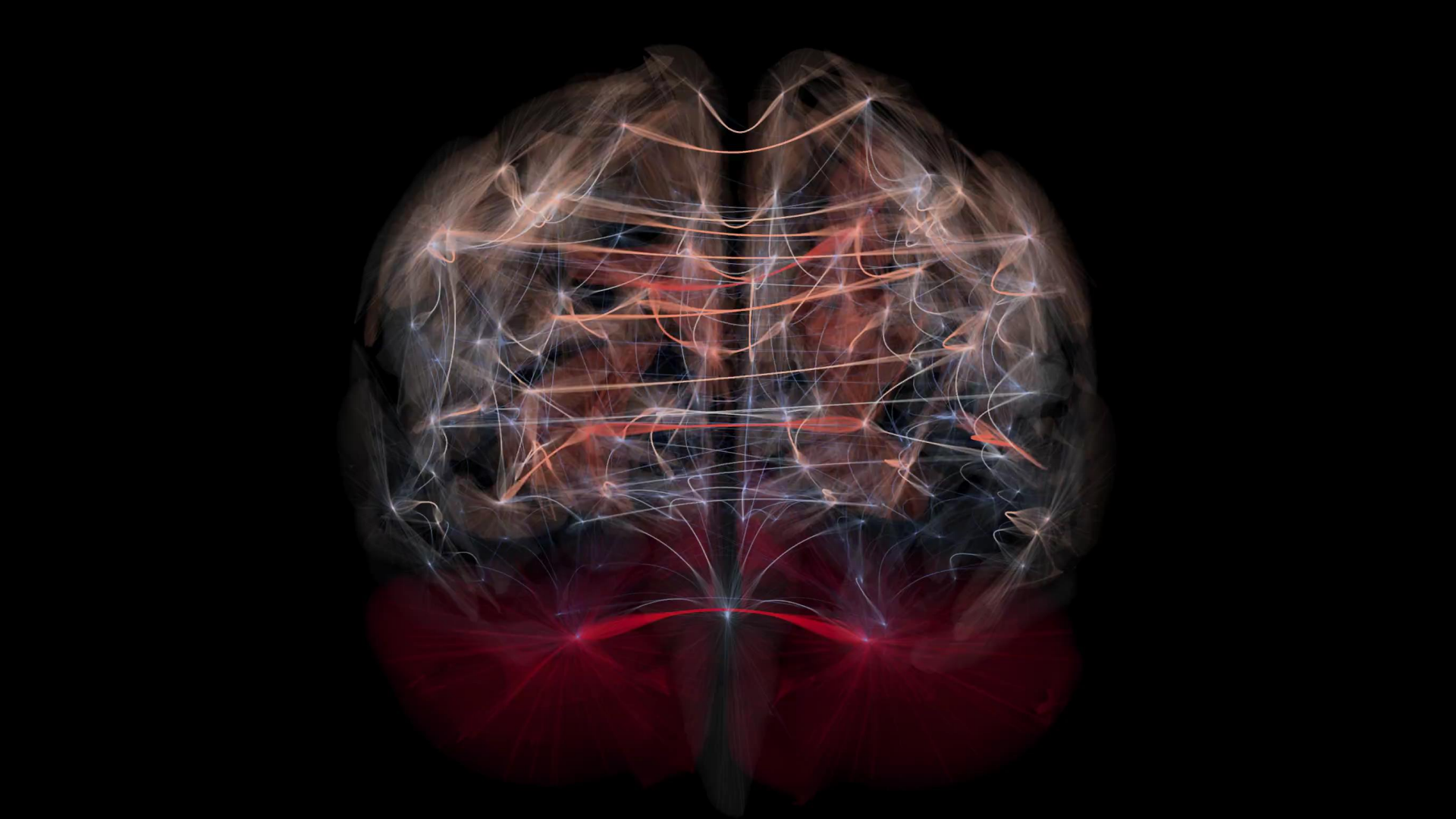
full dome hemispherical screen
negative pressure membrane screen
8x active 3D projectors (2560x1600 ea)
5.1 audio
4+1 workstation system

DomeLab

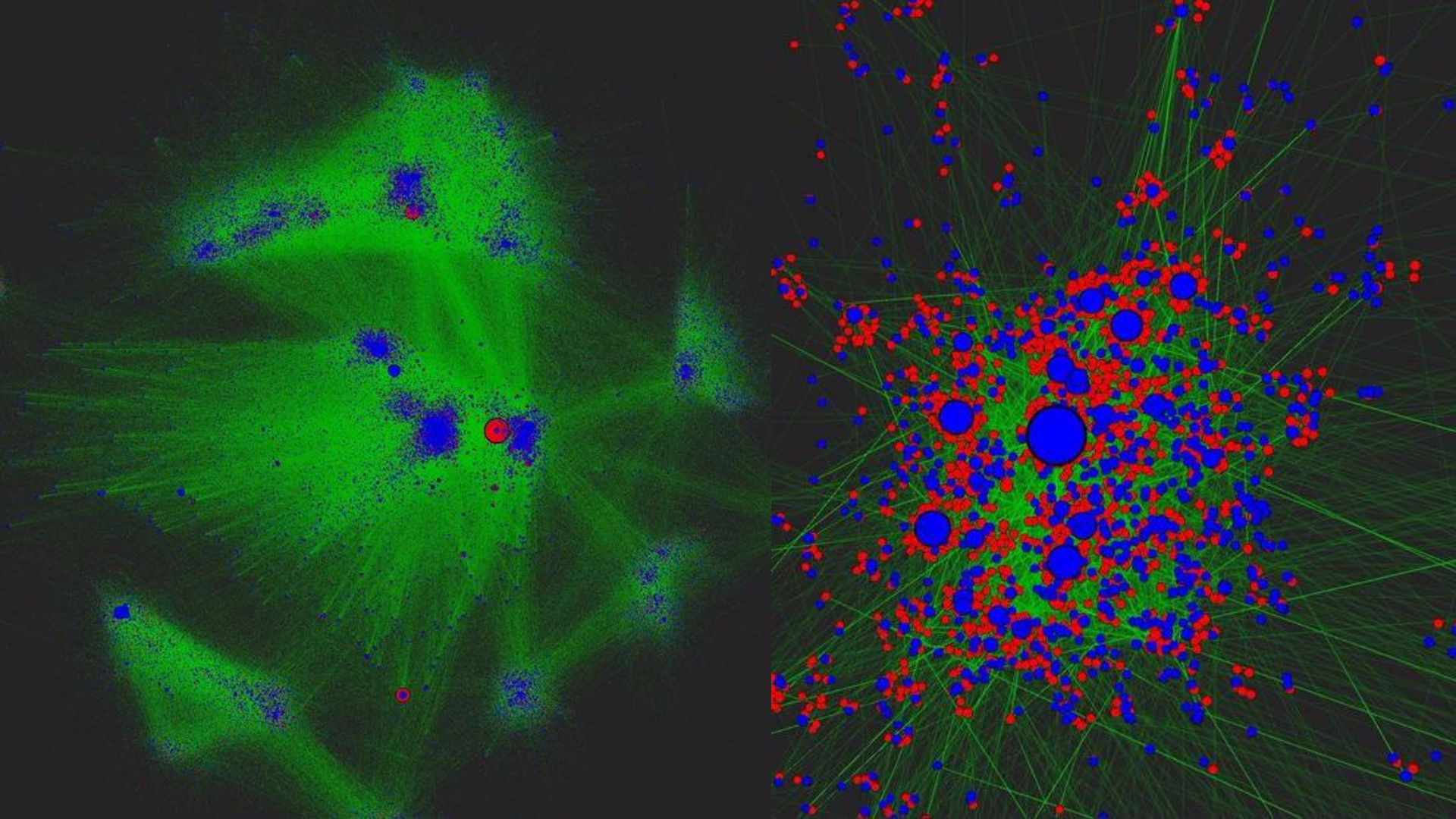


4K = 8 active 3D projectors
8+1 PC cluster
5.1 channels of sound





Genomics Viewer



2x Postdoctoral Fellows

EPICentre

UNSW Art & Design

- **One of Australia's leading research & teaching universities**
- **Vibrant campus life with a strong sense of community & inclusion**
- **Enjoy a career that makes a difference by collaborating & learning from the best**

At UNSW, we pride ourselves on being a workplace where the best people come to do their best work.

EPICentre (Expanded Perception & Interaction Centre) is a shared UNSW research centre located at the UNSW Art & Design campus. The Centre undertakes visualisation research in the fields of art, design, science, medicine and engineering as its mission statement. EPICentre's major research facilities are accessible to UNSW and external researchers. Government and industry users are also welcome. The staff of the Centre provide research collaboration, technical support, education and training to researchers accessing the facilities.

About the role

- 2 positions available
- Full time, fixed term appointments until 31 December 2019 at the following levels:
  - Level A annual salary between $73K - $98K, plus 9.5% super and leave loading; or
  - Level B annual salary between $103K - $121K, plus 9.5% super and leave loading.

The Postdoctoral Fellow will carry out innovative, impactful research that will lead to novel and important scientific and creative outcomes, including research integrating visualisation, simulations and computer graphics. The Postdoctoral Fellow will also be involved in research grants preparations and submission.

About the successful applicant

To be successful in this role you will:

- Doctoral qualifications in Computer Science, Engineering or a relevant field of study with a demonstrated track-record of science innovation and creativity and a willingness to contribute novel ideas and approaches to support scientific investigations.
- Proven experience conducting research in High Performance Computer Visualisation, Computer Vision, Image Analysis, Computer Graphics and Simulations.
- Experience building software in one of the following programming languages / frameworks: C/C++, C#, Python, OpenGL, OpenCL or CUDA, Vulkan.
- Experience in handling data scientific data sets including a demonstrated understanding of data management and analysis including emerging data curation standards; emerging data fusion methods, networked storage and (big) data processing, machine learning and simulation.

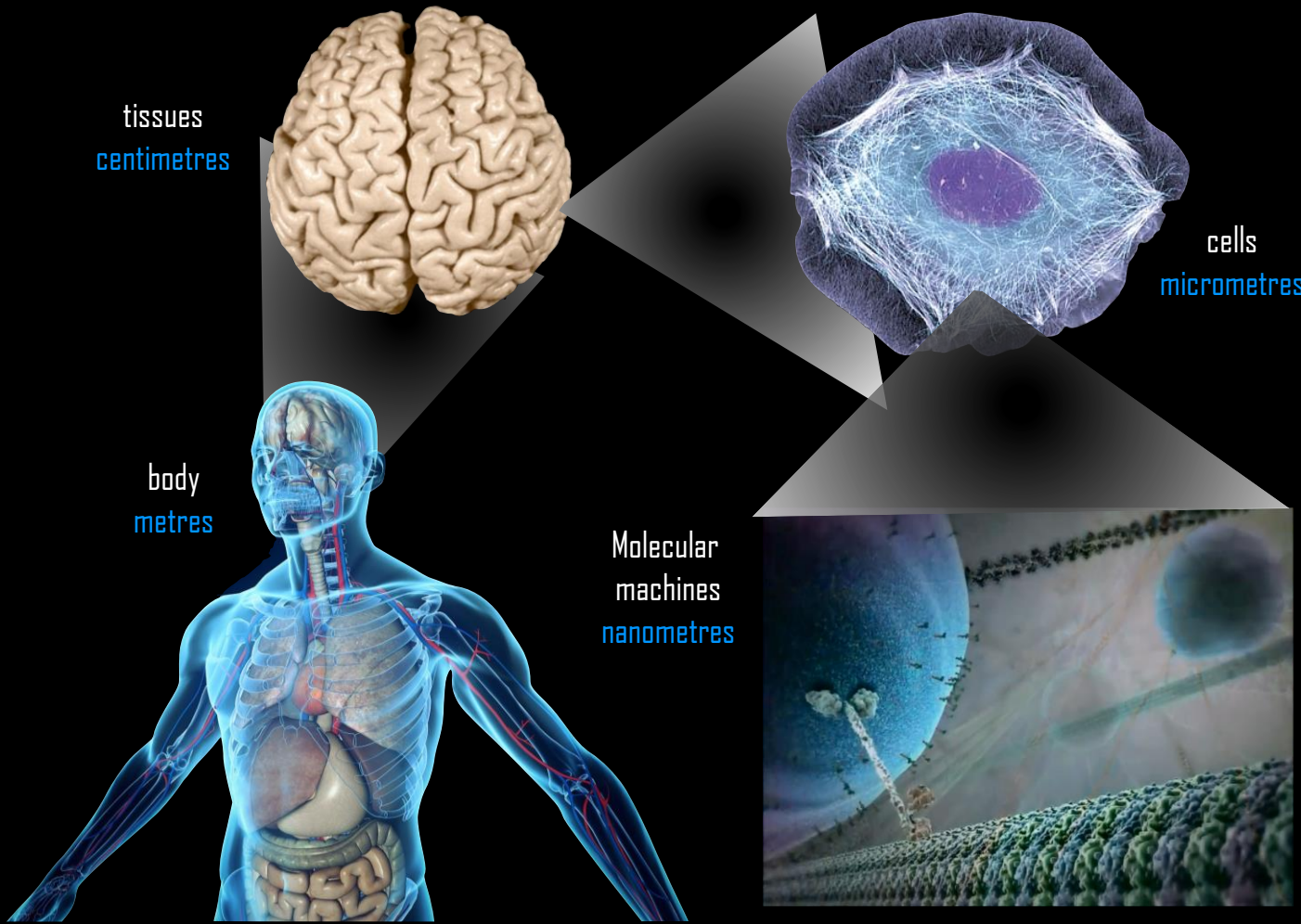
You should systematically address the selection criteria listed within the position description in your application. Please apply online - applications will not be accepted if sent directly to the contact listed.

Contact:

Associate Professor Tomasz Bednarz

E: t.bednarz@unsw.edu.au

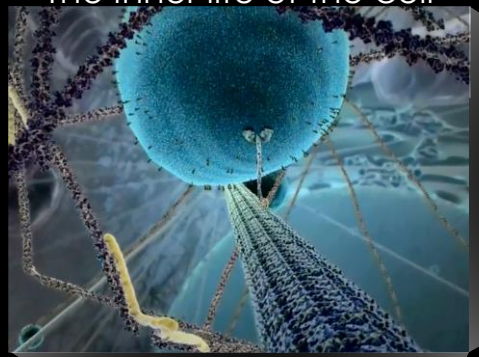
Life at small scales



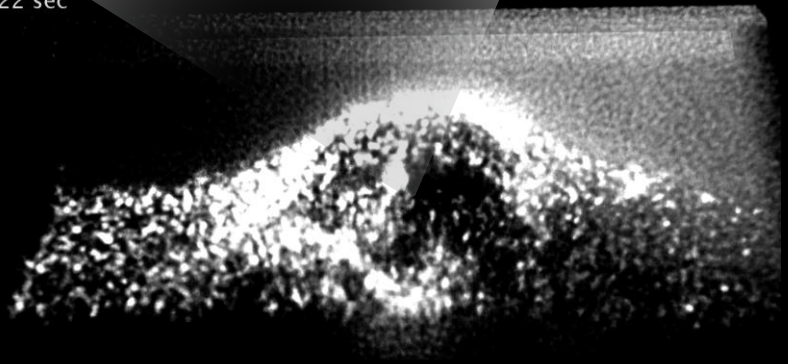
‘We know life by motion’

- Albert Szent-Györgyi

The inner life of the cell



22 sec

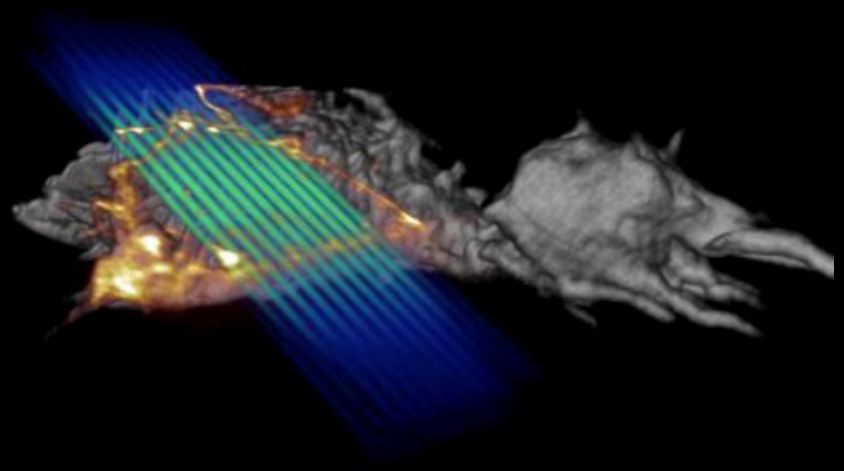


microtubule
growth rates ≈ 1μm/s

kinesins ≈ 0.8 μm/s

dyneins ≈ 1 μm/s

Volumetric imaging using a light sheet



series of 2D images (z,t)

↓

deskewed 3D images (t)

↓

4D data set of
cellular dynamics

↓

Image analysis

each volume of a cell = 50 - 100 images
typical time series: 1- 4 /s for 300 s

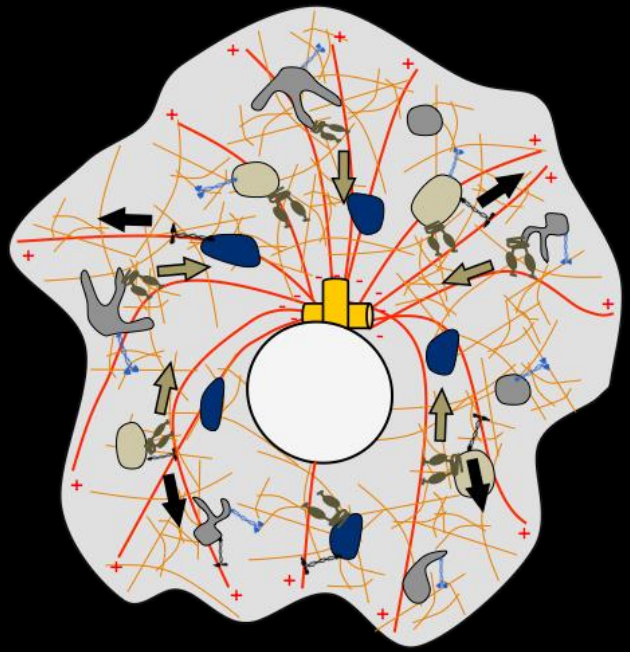
single cell, 4 colors: ~ 100 GB.

BC Chen et al., *Science*, 346:1257998, Oct. 24, 2014.

A city and a cell - understanding infections

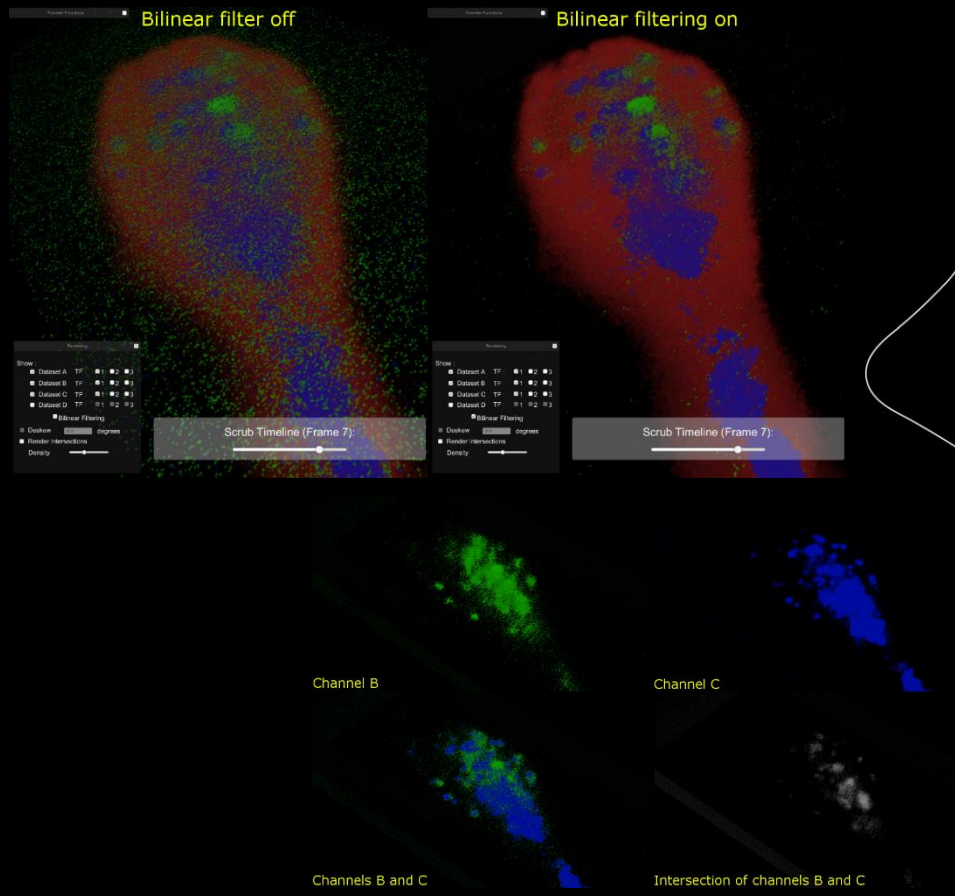
- What entities do infectious agents interact with?
- Where do they go when they attack?

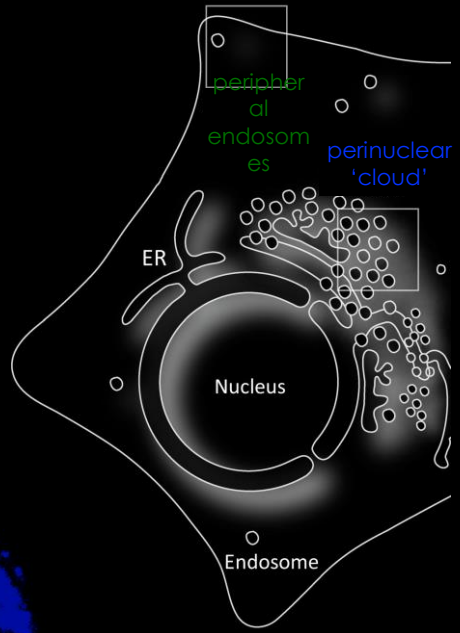
Mumbai seen from space - Astronaut Thomas Pesky - https://t.co/SltsVWnG8y

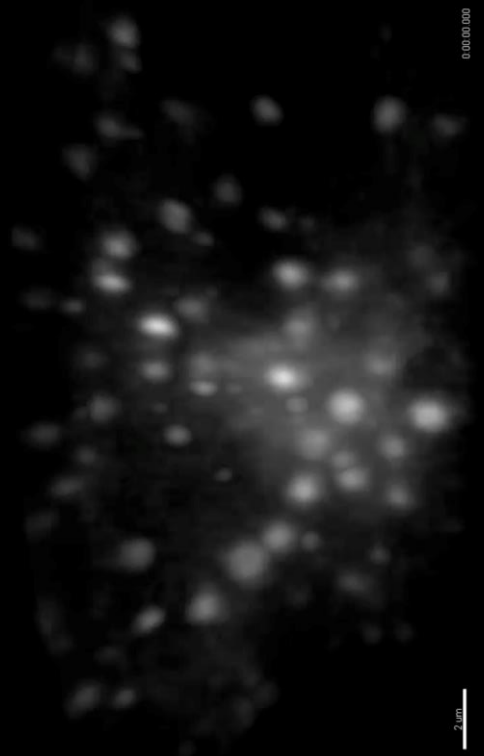


A simplified schematic of intracellular transport organization

Heterogeneous objects - tracking







Neefjes *et al.*, Trends in Cell Biol. 2017

Inspired Learning Initiative - Immersive Educational Experiences

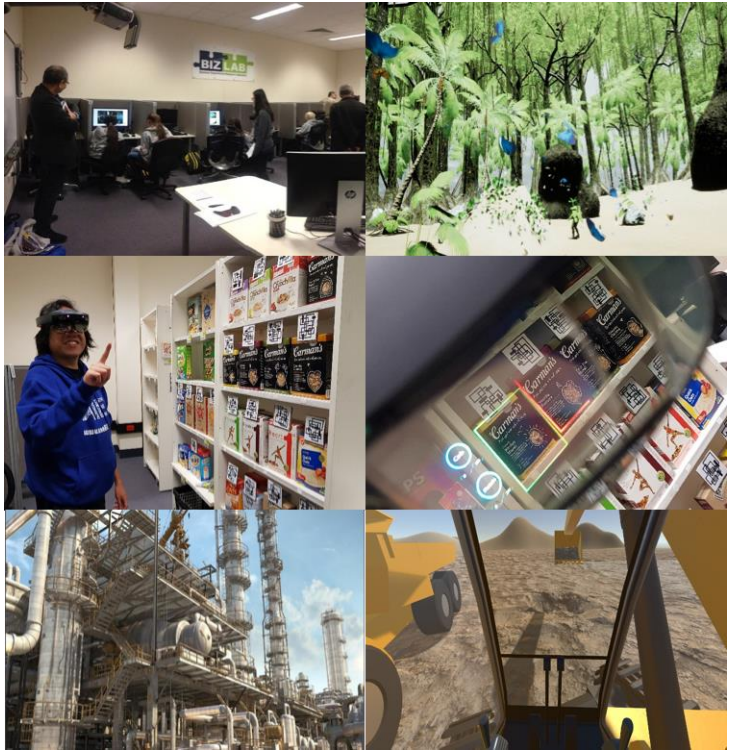
The Inspired Learning Initiative (AUD $77M) is a strategic grant that supports a 5-year program of work to improve and enhance the UNSW Scientia Education Experience. This Initiative is led and expedited by the Pro-Vice Chancellor (Education) portfolio (the central educational service hub for UNSW)

Digital Uplift - Redesign 660 courses

In year 1 (2017) of the Digital Uplift, the Immersive Experience Team delivered 15 AR/VR experiences using a variety of application and web-based learning objects embedded within courses.

Application-based examples include:

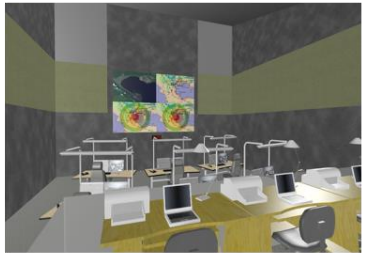
- Indigenous Astronomy (Torre Strait Islander Astronomy)
- Medical VR doctor (CPR experience)
- Marketing HoloLens (association of nutritional requirements)
- Construction VR (Operational safety)
- LIFESAVAR (Onsite safety)

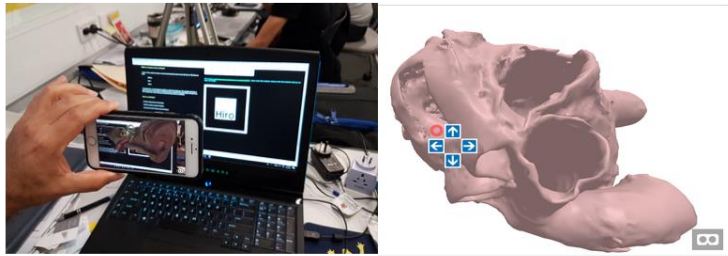


Inspired Learning Initiative - Immersive Educational Experiences

Web-based examples include:

- Psychology Phobias VR
- Medical Blood Donation VR
- Medical Empathy - Ophthalmology VR
- Medical Clinical Ethics VR
- Anatomy VR
- Situation Room Public Health VR
- Business - Superannuation VR
- Science - AR Geology
- Heart Anatomy VR
- AR Ear



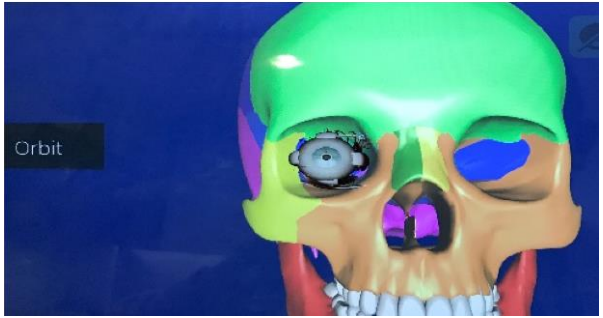


Students as Partners - Student Immersion

Student immersion to improve the educational value and experiences to support the design and development of educational offerings at UNSW Sydney

Program Overview
Students partnered with the PVCE portfolio to scale the design and development of immersive experiences including AR/VR/MR to enhance programs across UNSW Sydney.

2017 Student Partner Activity
30 students partnered with the PVCE portfolio across 9 projects.



Experimental Space at UNSW Art & Design

National Facility for Human-Robot Interaction Research

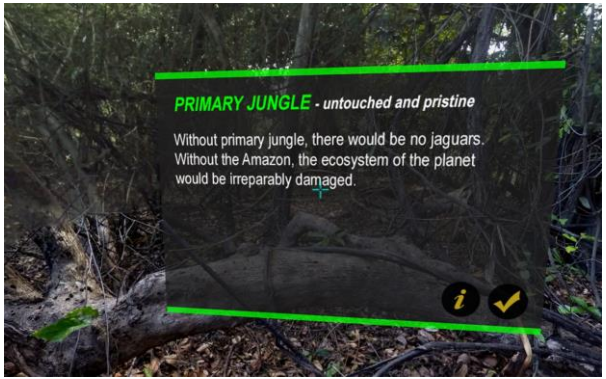
- Main experimental space: 16 metres x 7.5 metres, plus Waiting Room, Interview Room, Control Room and Server Room
- Highly instrumented: Over 190 discrete sensors
  - Pervasive visual and infrared spectrum imaging
  - Pervasive depth ranging
  - Pervasive audio pick-up
- Unobtrusively instrumented
  - Custom wall design obscures and de-emphasises sensor location
- Scriptable environmental controls
  - Lighting/sound/scent generator
- Fully functional kitchen for evaluating assistive robotics and rehabilitation
- Wheelchair accessible

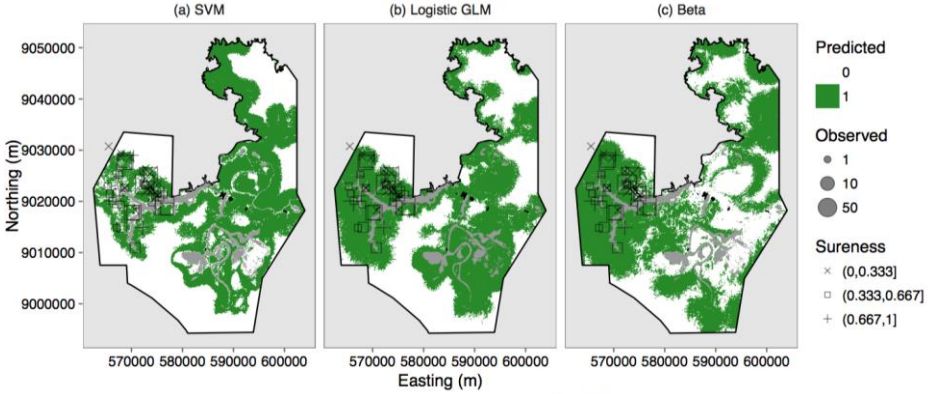
UNSW SYDNEY | THE UNIVERSITY OF SYDNEY | UTS UNIVERSITY OF TECHNOLOGY SYDNEY | ST VINCENT'S HOSPITAL SYDNEY

https://www.youtube.com/watch?v=Ti5rFSuk08M

Saving Jaguars – VR, Gaming, GPUs, Stats

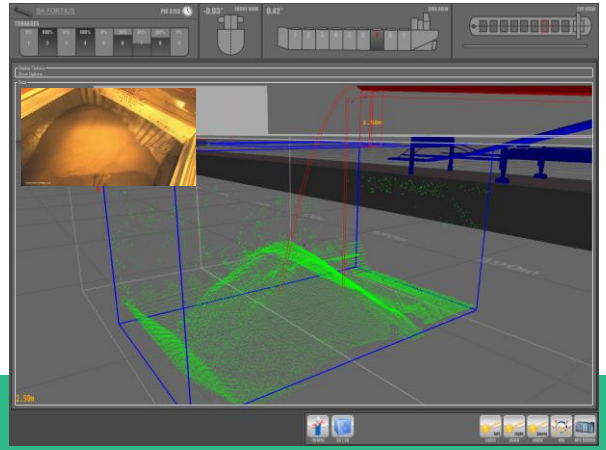
Saving Jaguars





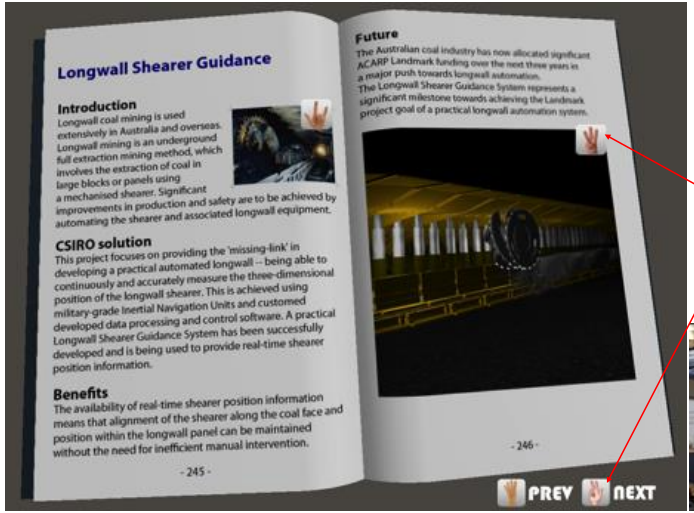
Visual Analytics for Mining

- Hemispherical dome
- Calibration software
- Remote data streaming

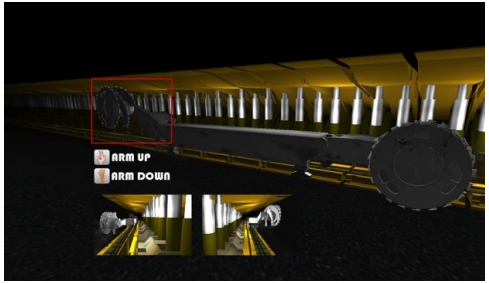


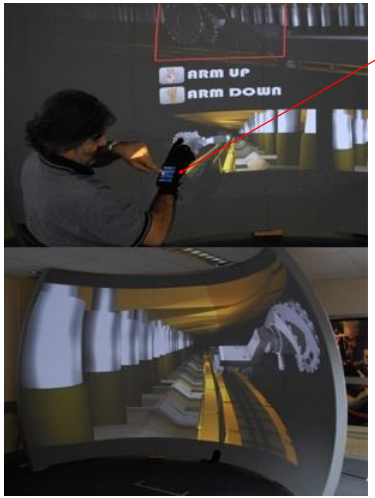
Immersive e-book

- Enhance e-Learning
- Experience interactions = remember more
- Test in class-room situations

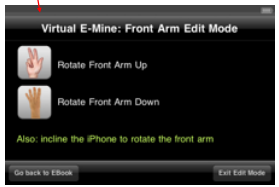


Hand gestures
to operate VR

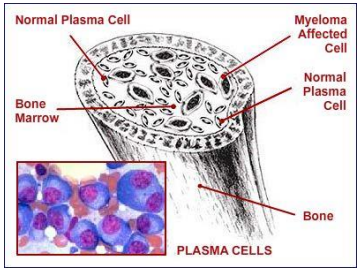




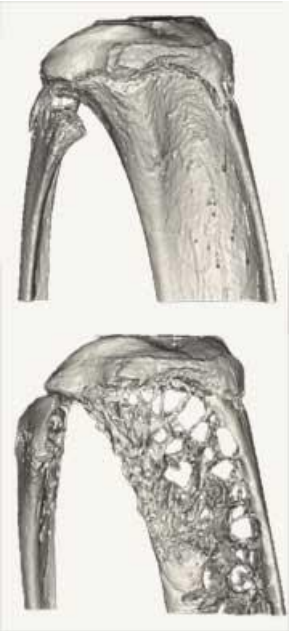
Use of iPhone's touch screen



Multiple Myeloma deadly cancer of blood plasma cells

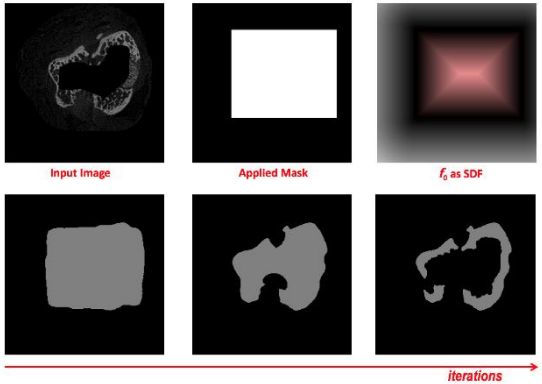


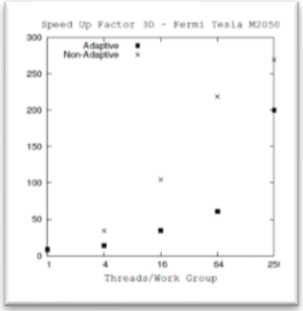
Collections of abnormal cells accumulate in bones, where they cause bone lesions (abnormal areas of tissue), and in the bone marrow where they interfere with the production of normal blood cells

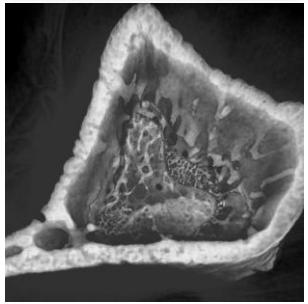


Governing equation / GPGPU compute

$$\frac{\partial f}{\partial t} = -\left|\nabla f\right|\left[aD(\bar{x}) + (1-a)\nabla\cdot\frac{\nabla f}{\left|\nabla f\right|}\right]$$

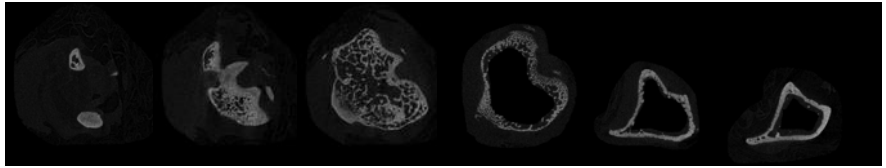


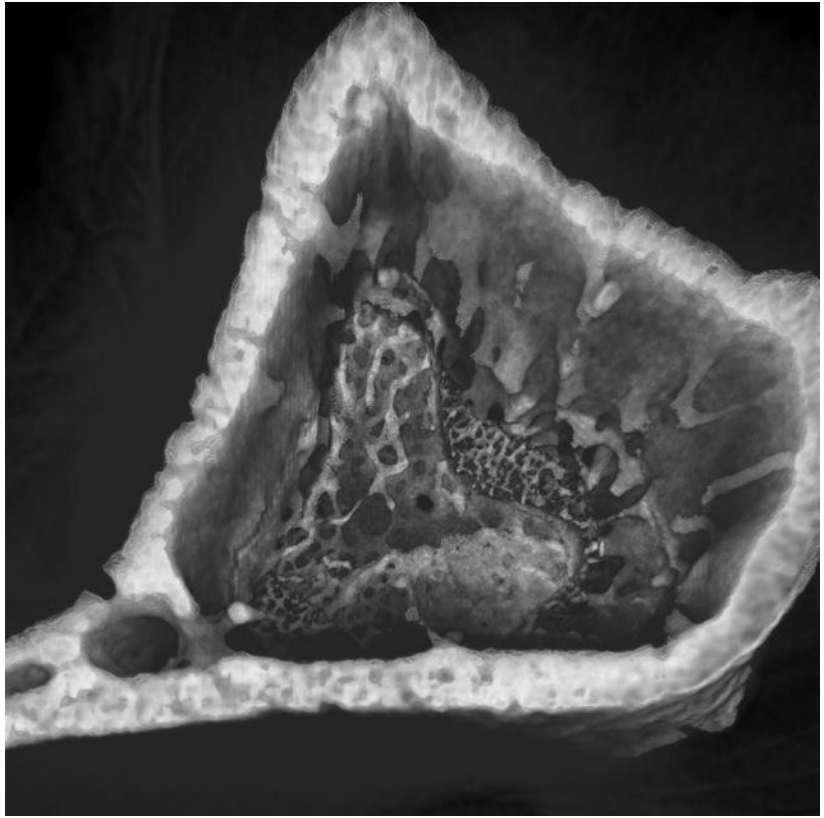




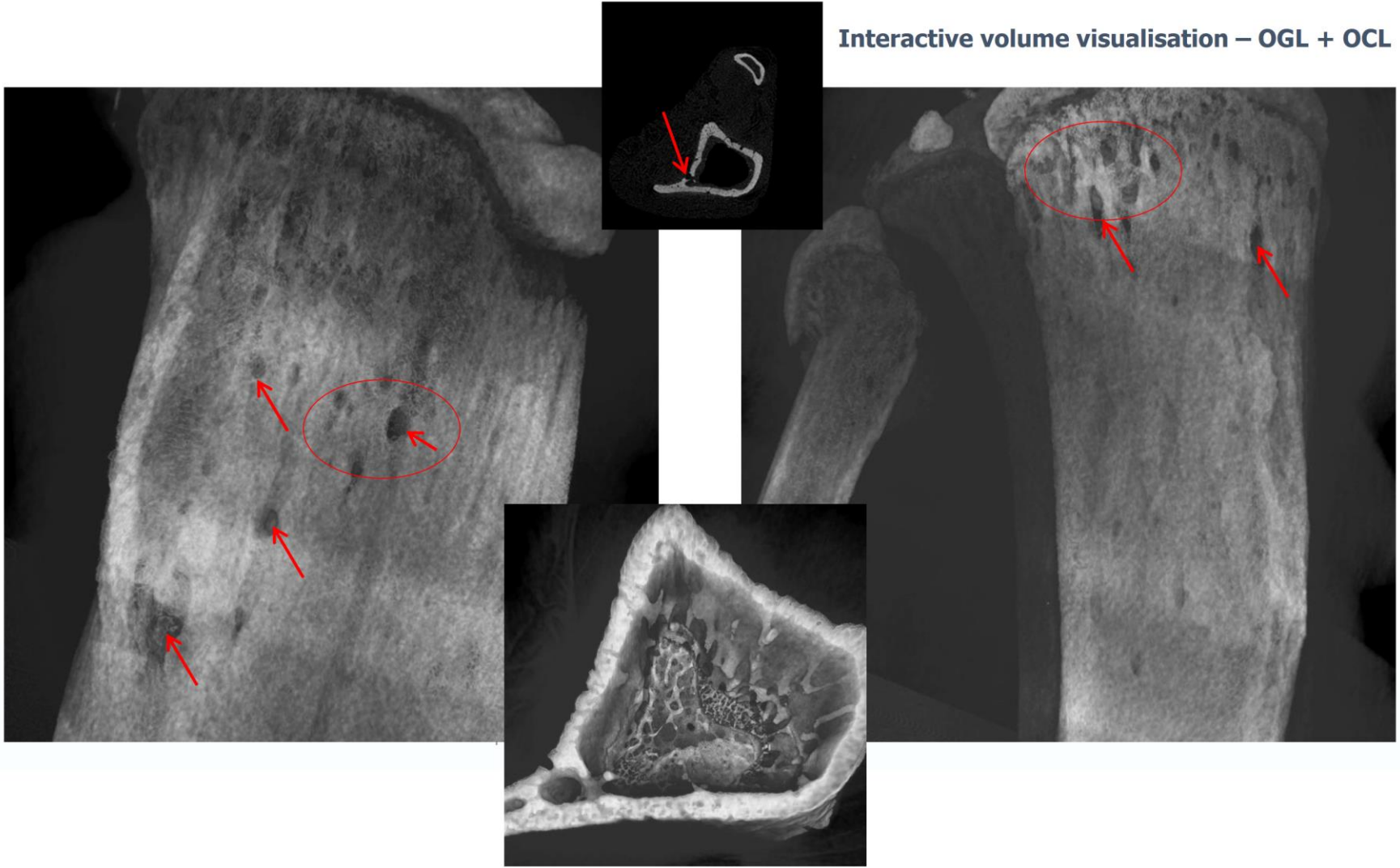
Bone Model c4-data-set

Interactive volume visualisation – OGL + OCL





Interactive volume visualisation – OGL + OCL



Siggraph Asia moves to Australia in 2019

MICE News

Wednesday, 22 March 2017

Asia's largest computer graphics conference and exhibition Siggraph Asia will be held in Brisbane, Australia in November 2019.

The event is expected to attract 6,000 of the world's top technical and creative talent across four days of discussions and demonstrations on emerging computer graphics and interactive techniques.

The successful bid to host the meeting and exhibition in Australia for the first time was a collaborative effort led by Brisbane Marketing with the conference component of the event delivering A$3.6 million in economic impact.

Brisbane will be promoted at the events editions in Bangkok (2017) and Tokyo (2018).

Brisbane Siggraph chapter chair, associate professor Tomasz Bednarz said: "Our mission is to make sure the Australasian region is activated, helping us to deliver a unique Siggraph experience in Brisbane. We will also be working to co-locate other events around the same time as the show to encourage the global graphics community to enjoy Australia."

See you in SIGGRAPH Asia 2019 Brisbane!

DATA 61

Thank you

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