

Imaging Atoms, Molecules and Cells

Imaging Atoms, Molecules and Cells

From a world of atoms
to a world of living matter

Dr Steve Barrett HWKU3A 31 Oct 2025

Introduction

A World of Atoms	Imaging atoms and molecules
Perception vs Reality	Why can image analysis be such a challenge?
The Spin-Offs	Applications in earth sciences and medical sciences
A World of Living Matter	Imaging more complex systems
Investigating Cancer	Spectromicroscopy and infrared absorption

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Introduction

This talk is about images and how we look at images in a scientific context. Two concepts are important in what follows:

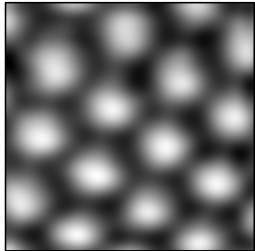
Image Processing	>>>	Interpretation
Image Analysis	>>>	Quantification

The talk will be illustrated with images from research projects old and new, from collaborators and from project students.

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A World of Atoms



On this scale, a grain of sand would be about the size of the Moon.

" To see a world in a grain of sand ... "

William Blake

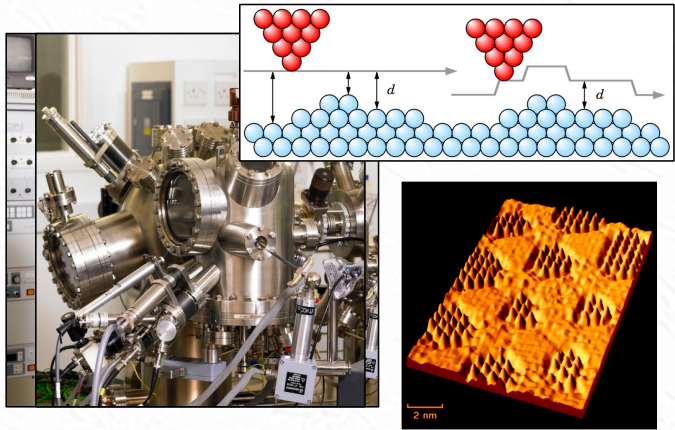
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World of Atoms

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A World of Atoms



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World of Atoms / Scanning Tunnelling Microscope

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A World of Atoms

Working with STM images led to the development of image analysis software that supports various scanning microscopy systems:

Scanning Tunnelling Microscope

Referring to any/all of these as SXM led to the unpronounceable:

Image SXM
v 2.05
December 2023
Steve Barrett



> 50,000 downloads in the past 10 years by universities and research centres

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World of Atoms / STM / Software

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Image SXM

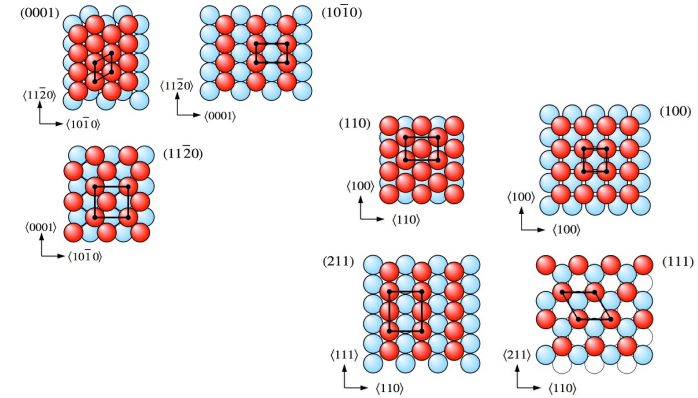


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World of Atoms / STM / Software / Image SXM

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A World of Atoms



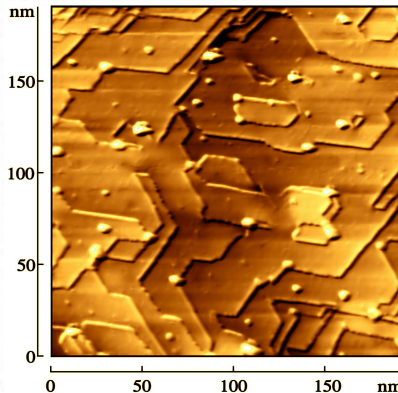
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World of Atoms / STM / Surface Structure

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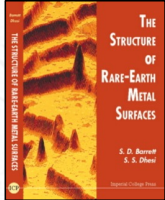
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A World of Atoms



Sc(0001)

For many years I studied the rare-earth metals using a combination of spectroscopy, microscopy and diffraction techniques

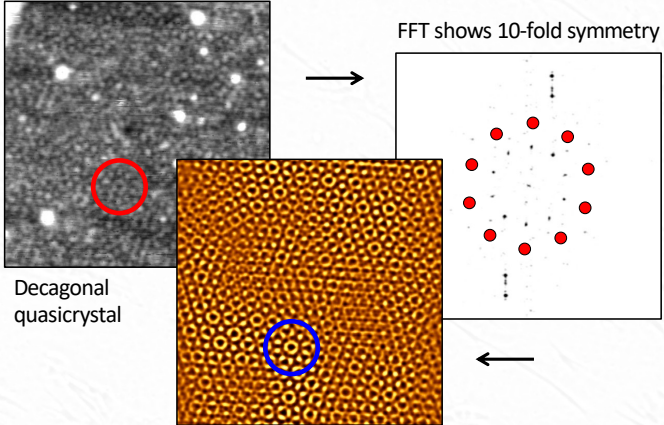


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World of Atoms / STM / Surface Structure / PRB 51 (1995) 17946

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A World of Atoms



Decagonal quasicrystal

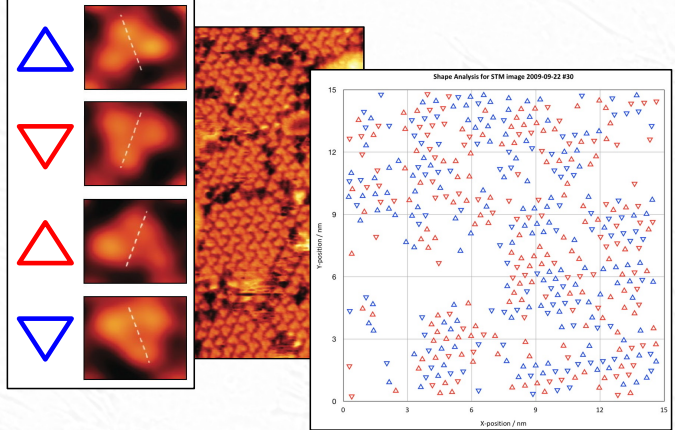
FFT shows 10-fold symmetry

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World of Atoms / STM / Quasicrystals / PRMS 40 (2005) 215

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A World of Atoms



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World of Atoms / STM / Molecules / JPC C 115 (2011) 1180

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Astrophotography



The Milky Way from Kenya.
Due to the dark skies, very little image processing is required.

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Beyond Microscopy / Astrophotography

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Astrophotography

NGC7000 North America Nebula



Single raw image

However, under the light-polluted skies of the UK, image processing can bring out hidden structures in a faint nebula.



Astrophotography

NGC7000 North America Nebula



Single raw image

20 Images stacked in Image SXM

Colours enhanced



A World of Atoms

Imaging atoms
and molecules

Perception vs Reality

Why can image analysis
be such a challenge?

The Spin-Offs

Applications in earth sciences
and medical sciences

A World of Living Matter

Imaging more
complex systems

Investigating Cancer

Spectromicroscopy and
infrared absorption



Perception vs Reality

How we perceive images (what we **see**) can be VERY different from the actual information content (what is **there**). In most day-to-day situations we trust the former and don't worry about the latter.

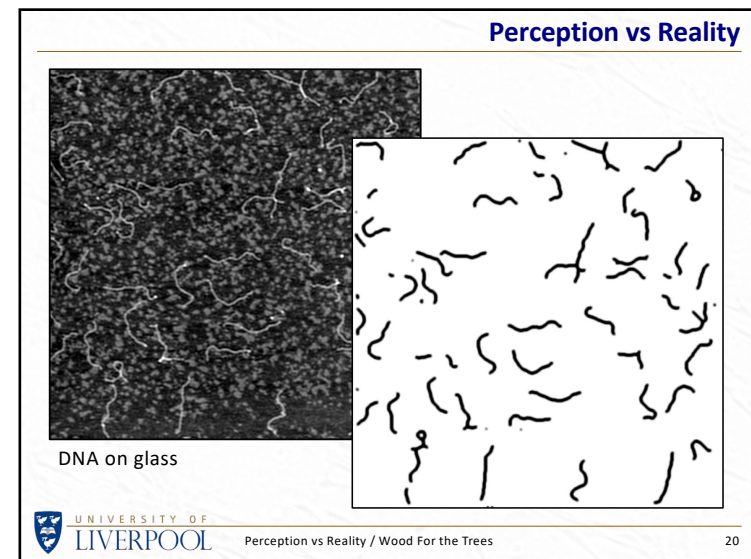
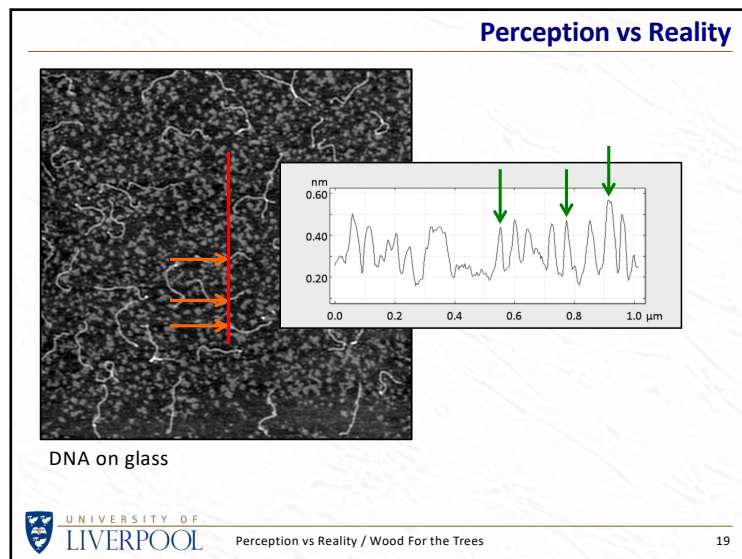
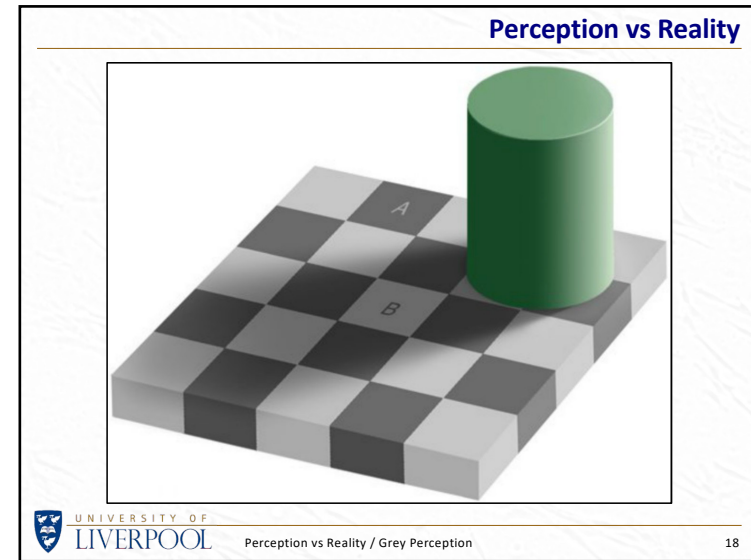
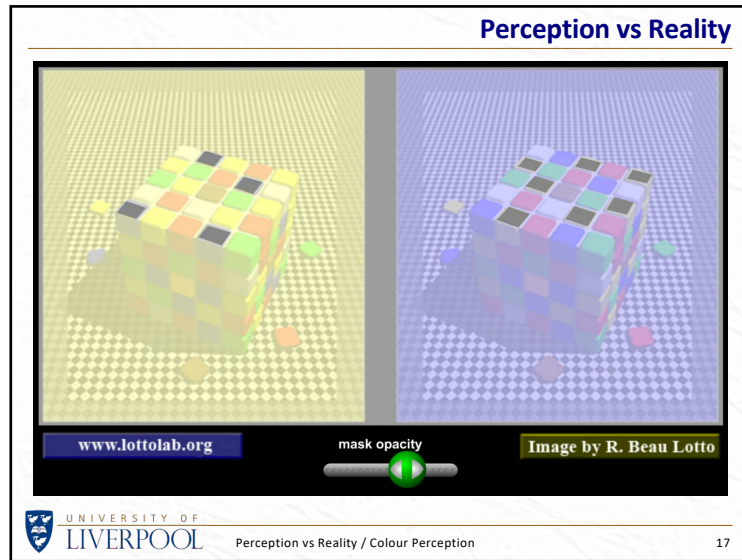
Which is the better image processor?

Brain vs **Computer**

Carbon vs **Silicon**



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Spin-Offs

A World of Atoms

Perception vs Reality

The Spin-Offs

A World of Living Matter

Investigating Cancer

Imaging atoms and molecules

Why can image analysis be such a challenge?

Applications in earth sciences and medical sciences

Imaging more complex systems

Spectromicroscopy and infrared absorption

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Spin-Offs

Applications to disciplines beyond physics and chemistry were a natural consequence of the interdisciplinary nature of image analysis. In particular...

Earth Sciences

'Principles of Computer Integrated Polarisation Image Analysis'

Medical Sciences

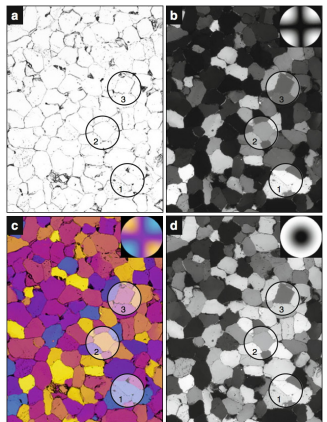
'Microscopy Image Analysis Software for Medical Applications'

PrinCIPia

MIASMA

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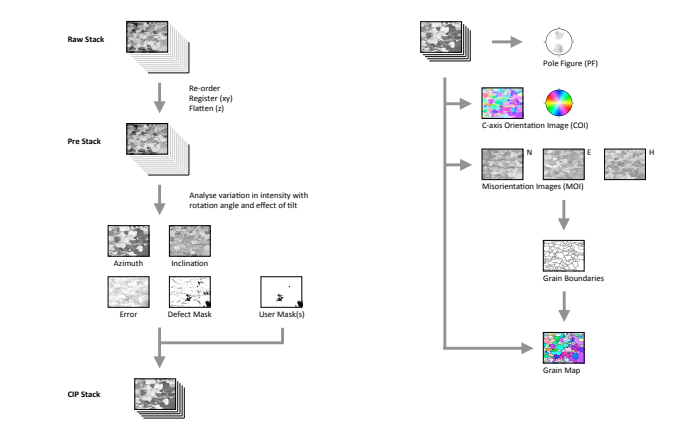
Earth Sciences



Imaging earth materials (to a physicist = 'rocks') using circularly and linearly polarised light produces colours and intensities that depend on the orientation of the crystallographic axes of the grains with respect to the optical axis of the microscope.

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PrinCIPia



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PrinCIPIa

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Spin-Offs / Earth Sciences / PrinCIPIa

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Earth Sciences

Ongoing collaboration with Professor Heilbronner at the University of Basel led to a book on Image Analysis ...
... available at a reasonable price from the author.

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Spin-Offs / Earth Sciences

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Medical Sciences

Medical spin-offs have expanded considerably in the past ten years:

MIASMA What is MIASMA? What can MIASMA do? Particulates Parasites Circulation Retinas	Morphology Lymphocytes Lipid Bodies Microfibrils Bacteria
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Spin-Offs / Medical Sciences / MIASMA / Acta Bio. 10 (2014) 4843

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Human Chromosomes

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Spin-Offs / Medical Sciences / Chromosomes

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A World of Atoms

Imaging atoms and molecules

Perception vs Reality

Why can image analysis be such a challenge?

The Spin-Offs

Applications in earth sciences and medical sciences

A World of Living Matter

Imaging more complex systems

Investigating Cancer

Spectromicroscopy and infrared absorption

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A World of Living Matter

Now very much in the world of living matter, we take a closer look at two research projects in which image analysis played a key role:

Microcirculation Analysis

Investigation of Cancer

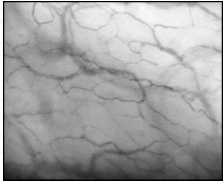
World of Living Matter30

Microcirculation Analysis

In collaboration with consultants at Alder Hey hospital, the first trials of *MIASMA* software were conducted on patients in the intensive care unit. Some of these patients suffered from meningitis, causing sepsis (aka blood poisoning).

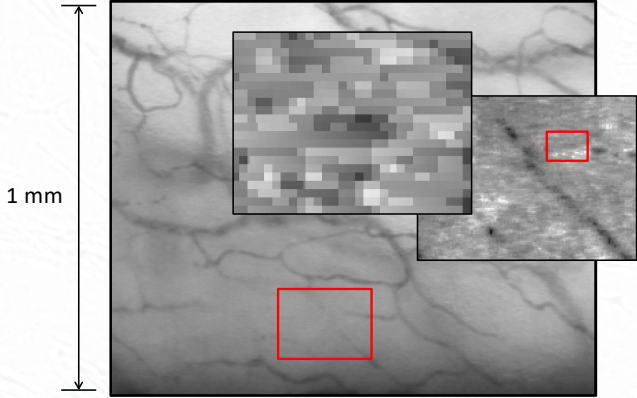
The software quantified the flow of blood cells through a capillary network, the *microcirculation*, as imaged by a small portable microscope placed underneath the tongue of the patient.

Not so much
Putting People Under the Microscope
but rather
Putting the Microscope Under People.



World of Living Matter / Microcirculation Analysis31

Microcirculation Analysis



World of Living Matter / Microcirculation Analysis32

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Microcirculation Analysis

Bear in mind that the blood vessels are invisible (as only the blood cells, containing haemoglobin, are imaged).

So the problem is to identify and quantify the motion of a blood cell relative to an invisible vessel in a sequence of video images that are not stable – ever tried to get a five-year old to sit still while you place a microscope under his tongue?

Any attempt at quantification will first have to deal with ...

... Translation ... Magnification ... Rotation ... Distortion ...

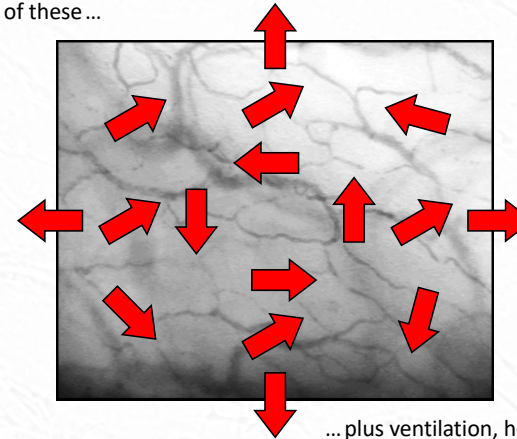


World of Living Matter / Microcirculation Analysis

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Microcirculation Analysis

Or all of these ...



... plus ventilation, heartbeat

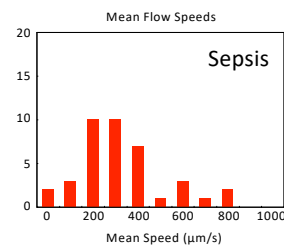
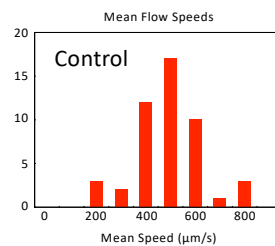


World of Living Matter / Microcirculation Analysis / Video Stability

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Microcirculation Analysis

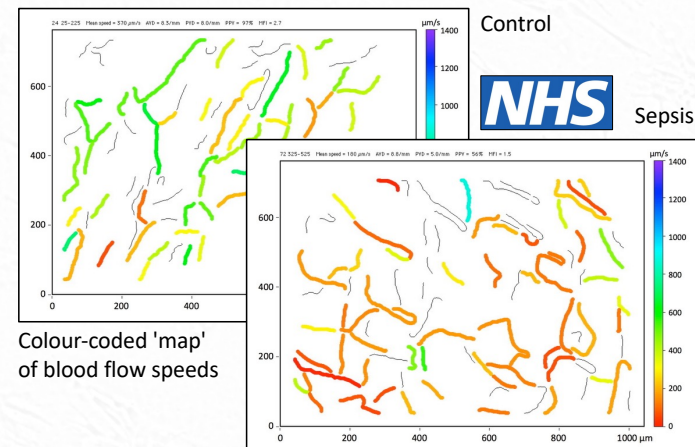
Through a combination of techniques, including cross-correlations (to stabilise the video images) and autocorrelations (to identify the motion of blood cells that are barely detectable) it is possible to quantify the blood flow speeds in vessels as small as 7 μm diameter.



World of Living Matter / Microcirculation Analysis

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Microcirculation Analysis



World of Living Matter / Microcirculation Analysis

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Imaging Atoms, Molecules and Cells

A World of Atoms Imaging atoms and molecules

Perception vs Reality Why can image analysis be such a challenge?

The Spin-Offs Applications in earth sciences and medical sciences

A World of Living Matter Imaging more complex systems

Investigating Cancer Spectromicroscopy and infrared absorption

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Investigating Cancer

This final section of the talk describes research funded through EPSRC, CRUK and NIHR research grants.

The main aim is to answer the question...

Can we identify an infrared absorption signature for tissue that is likely to become cancerous?

Or ...

Can we detect cancer before it is cancer?

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World of Living Matter / Investigating Cancer

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Free-Electron Laser

ALICE was an accelerator at Daresbury Laboratory that was an intense source of infrared light with a frequency of THz.

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World of Living Matter / Investigating Cancer / SNOM / ALICE FEL

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Free-Electron Laser

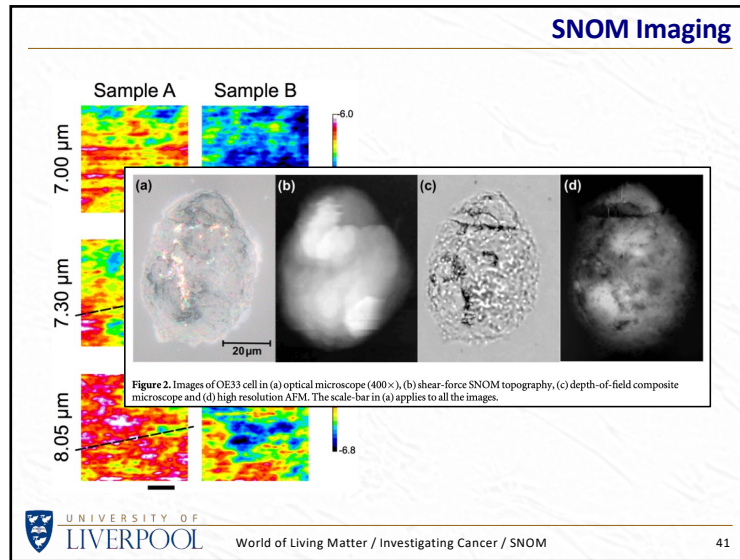
An array of magnets with alternating N-S orientation causes the electron beam to 'wobble' and emit intense beams of synchrotron radiation. The strength and period of the magnet array determines the wavelength of the emitted radiation.

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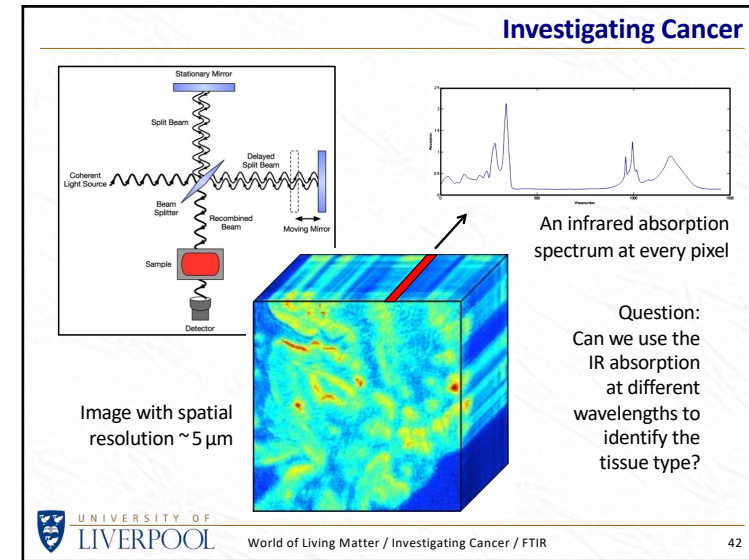
World of Living Matter / Investigating Cancer / SNOM / ALICE FEL

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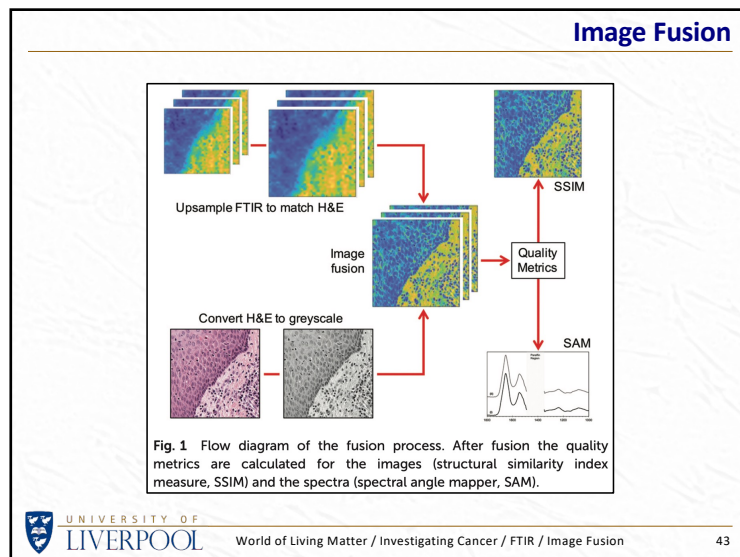
Imaging Atoms, Molecules and Cells



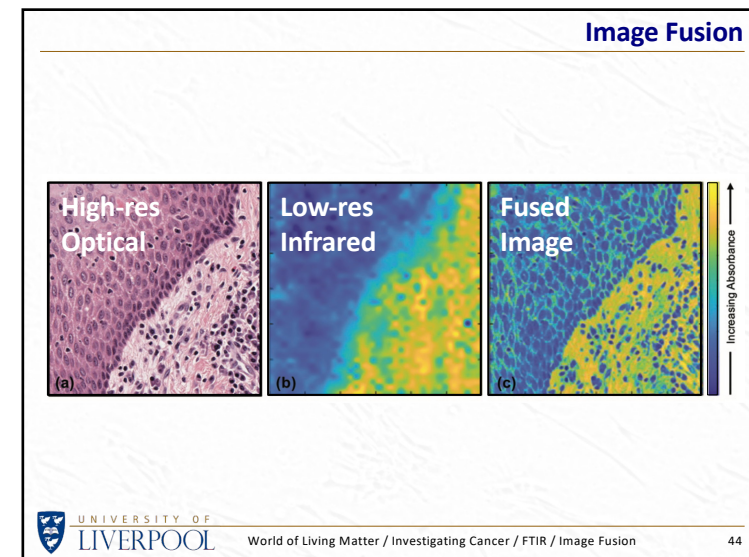
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Tissue Types

What type of tissue are we studying?

Epithelium tissue covers all surfaces of the human body. This means not just your skin ...

... but also the oesophagus and mouth.

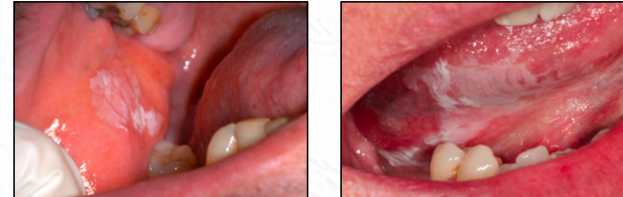


After studying oesophageal cancer cells we are now focussing on oral epithelial dysplasia (OED) – changes in the cells that make up the lining of the mouth.

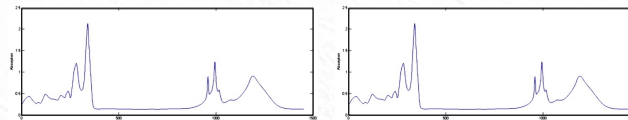
In particular, we want to improve the accuracy of prognosis so that we can say if a lesion found in the mouth will, or won't, progress to cancer.

Transforming or Non-Transforming?

Two oral lesions ... one will transform to cancer, the other won't.

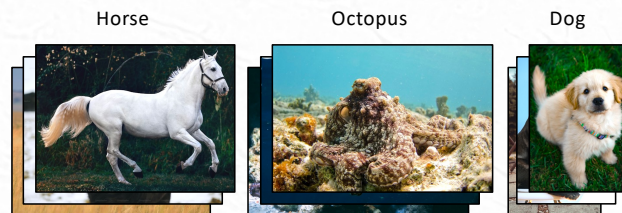


But which is which?



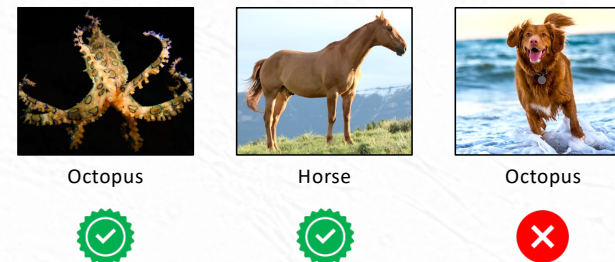
Artificial Intelligence

Training AI



Artificial Intelligence

Validating AI



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LDIR Wand



SciaScan
Spectro Chemical Infrared Analysis Scan For Cancer







World of Living Matter / Investigating Cancer / LDIR Wand

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Summary

A World of Atoms	Imaging atoms and molecules
Perception vs Reality	Why can image analysis be such a challenge?
The Spin-Offs	Applications in earth sciences and medical sciences
A World of Living Matter	Imaging more complex systems
Investigating Cancer	Spectromicroscopy and infrared absorption



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Acknowledgements

UoL staff
David Martin, Andy Wolski

UoL students
Safaa Al Jedani, Thiazzi Anakrazia, Tim Craig, Barney Ellis, James Ingham, Marion Leibl, Sean Littlewood, Graham Smith, Conor Whitley

SCAnCan Collaboration
Michele Siggel-King (UoL)
Antonio Cricenti, Marco Luce (Rome)

SciaScan Collaboration
Paul Harrison, James Ingham, Caroline McCarthy, Janet Risk, Richard Shaw, Caroline Smith, Asterios Triantafyllou, Paul Unsworth, Peter Weightman

ASTeC staff
Mark Surman
Neil Thompson

MIASMA
Riaz Akhtar, Laura Burgess, Enitan Carroll, Rebecca Clements, Liz Laird, Luning Liu, Naga Puppala, Richard Sarginson, Richard Wilkes, Yalin Zheng

PrinCIPIa
Renée Heilbronner, Rüdiger Kilian





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www.liverpool.ac.uk/~sdb/Talks

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