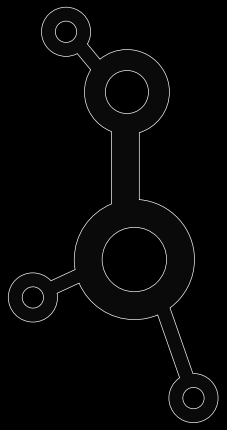


iMEC

VISUALISATION

THE ART AND SCIENCE OF INSIGHT IN RESEARCH

INDEX

FOREWORD

As researchers become more ambitious and the quality of research sensors become increasingly proficient, finding new ways to process, analyse and interpret larger volumes of more complex data requires increasingly elaborate infrastructure and most importantly the skilled operators to assist researchers to 'make meaning' of this valuable resource.

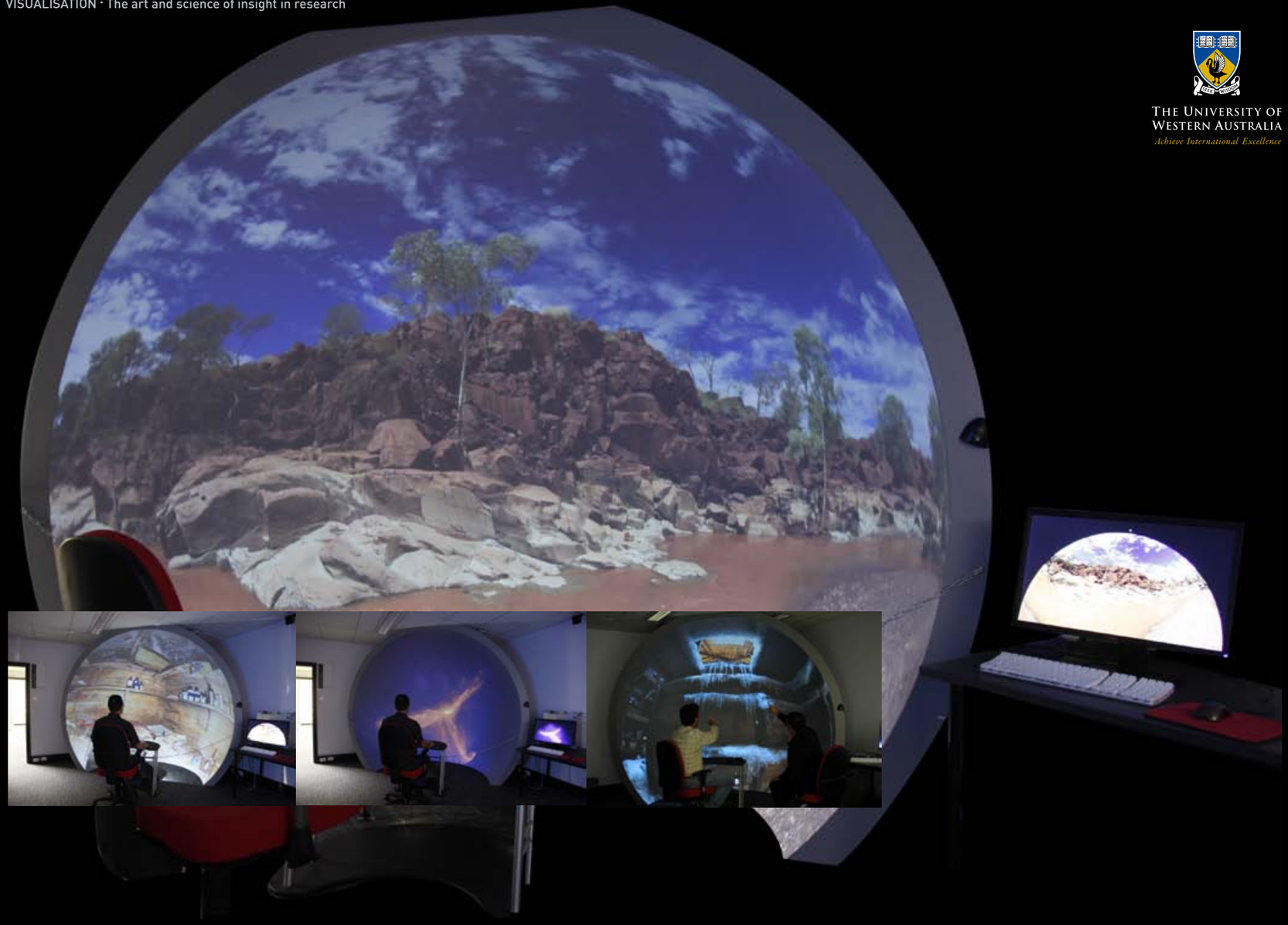
iVEC, along with the rest of the Australian research community, is continuing to build its visualisation capabilities; both physical and human. Through this collection, iVEC wishes to share some of the quite spectacular work that is being done across the Australian research community using iVEC infrastructure.

Hon Dr Mal Bryce AO
iVEC Chairman

INTRO

Visualisation applies advanced computing techniques to data in order to provide the researcher with insight into the underlying structures, relationships, and processes. As such, visualisation finds applications across a wide range of disciplines especially those with datasets that are large or contain complicated relationships. While visualisation may employ other senses such as hearing (signification) and touch (haptics), the predominant means of communicating with the human brain is through the sense of sight. The resulting visual outcomes can be employed for a range of purposes, sometime they are only applicable to the researcher and their peers, but often they can be used to convey and inform a wider audience. Occasionally the results are visually appealing and can further engage a general audience with the underlying research topic. This book presents examples of the later, images arising from visualising science across a number of disciplines and the iVEC partners.

Associate Professor Paul Bourke
UWA Facility Director



The University of Western Australia
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IDOME

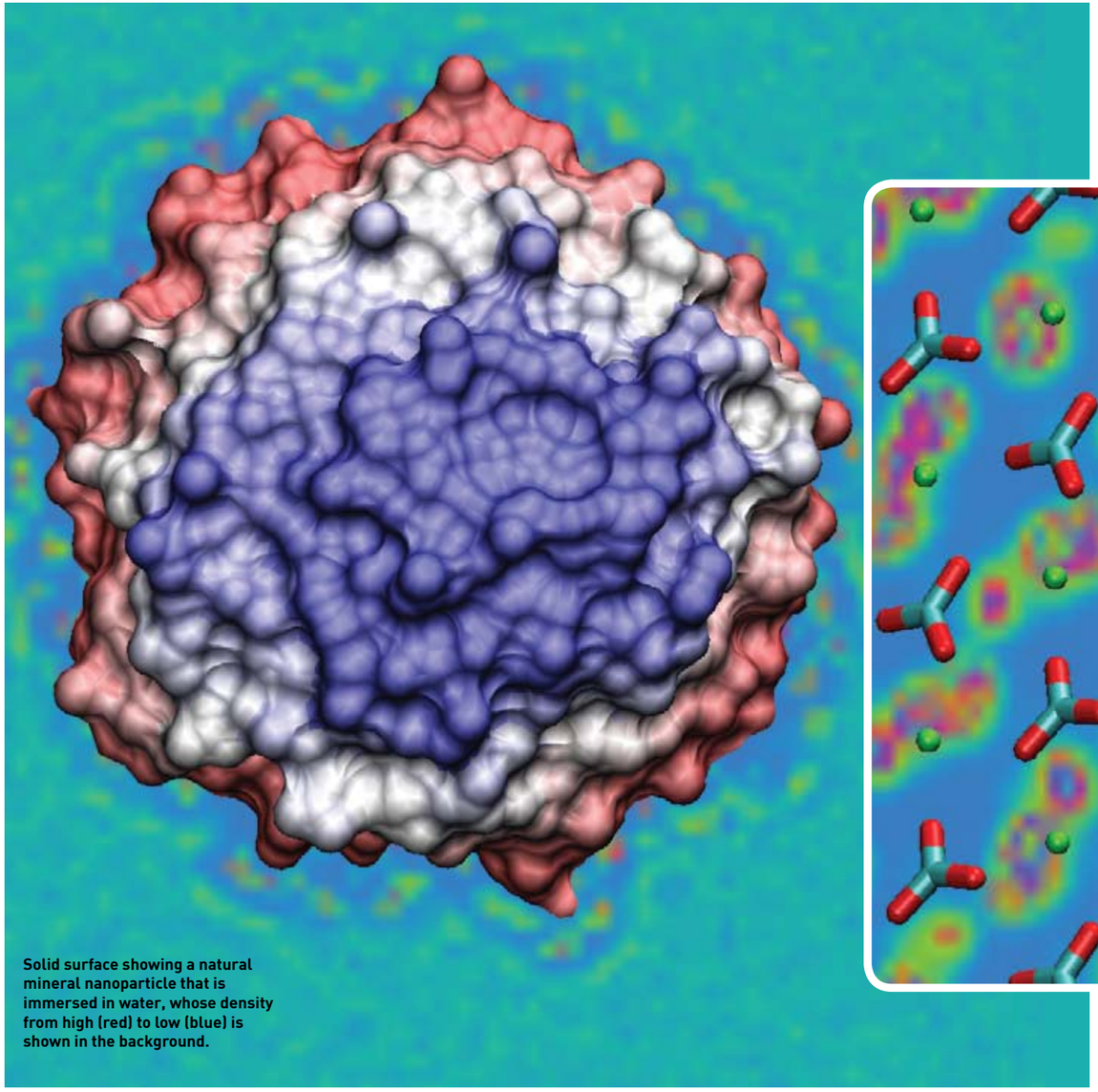
Project leader

Paul Bourke

Project Overview

Visualisation, as the name suggests, most often uses the sense of vision to convey information to the human brain. It would seem reasonable to try and exploit the full capabilities of that sense and therefore visualisation often uses novel display technologies to present data to the researcher. Stereoscopic 3D displays leverage the depth perception we enjoy when viewing the real world with two eyes and can assist with an understanding of spatial relationships in geometrically complicated datasets. High resolution displays, sometimes tiled, are utilised to view large detailed data making use of the visual acuity of the eye that is generally higher than standard digital displays or projections. The third characteristic of our visual system is peripheral vision, that is, even when looking directly ahead we can sense objects at almost 90 degrees to the left and right and about 60 degrees above and below.

The iDome is one of a number of displays that fills the viewer's visual field of view. In most traditional displays the digital world is framed with the border of the display, firmly anchoring it in the real world. The so called "removing the frame" of immersive displays such as the iDome gives the viewer a stronger sense of "being there". An interesting side effect of immersive displays is they can often convey a sense of depth without explicitly presenting stereoscopically. When the visual field no longer has a frame of reference (border) the brain uses other depth cues such as relative motion to construct depth information. Applications of the iDome include presenting and visualisation within virtual worlds, such as in virtual heritage and architecture. For scientific data it is usually employed in cases where one would like to explore the data structure from the inside, as opposed to the more usual views from the outside.

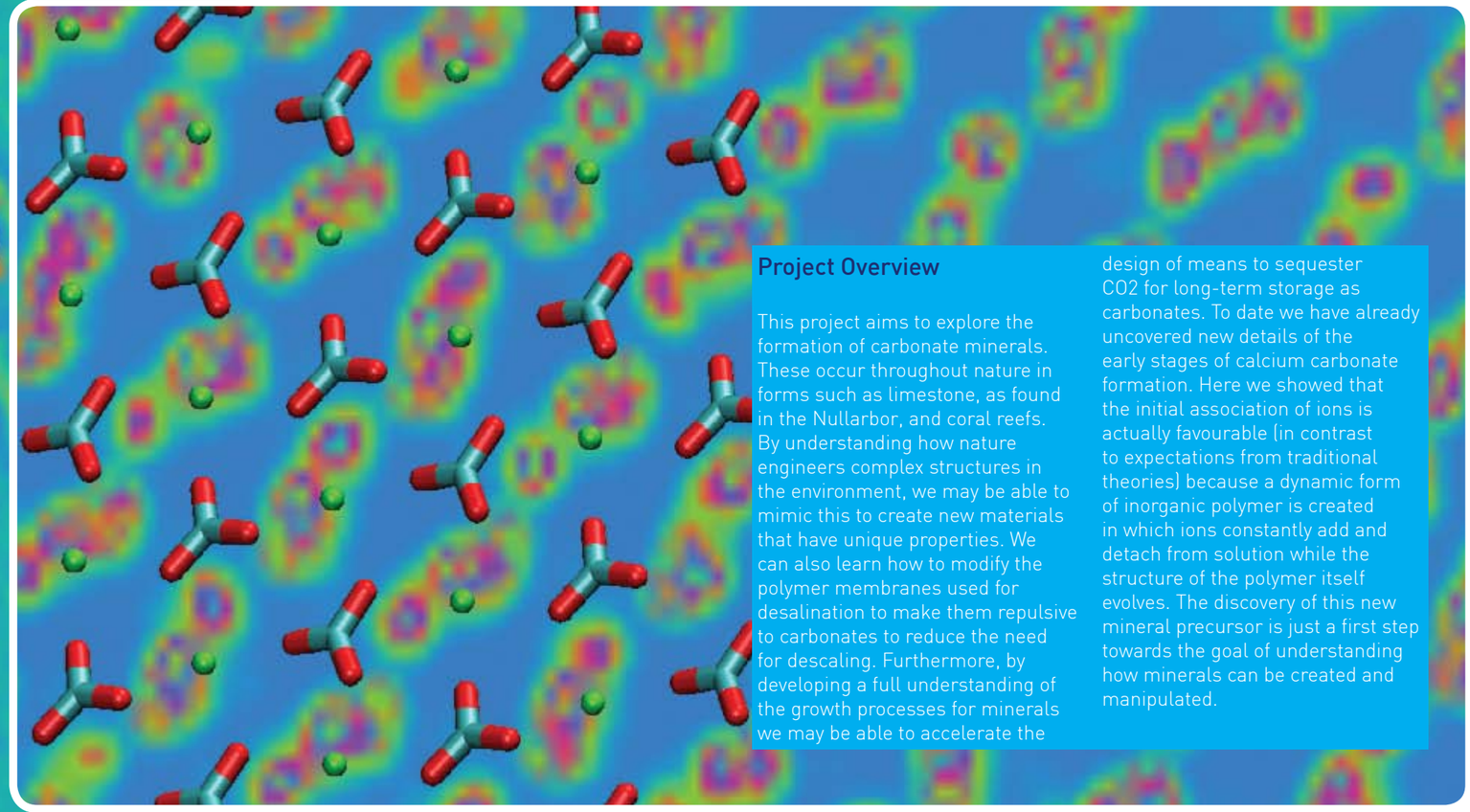


Solid surface showing a natural mineral nanoparticle that is immersed in water, whose density from high (red) to low (blue) is shown in the background.

Curtin University

ATOMISTIC SIMULATION OF MINERALS AND GEOCHEMISTRY

Project leader
Prof. Julian Gale



Project Overview

This project aims to explore the formation of carbonate minerals. These occur throughout nature in forms such as limestone, as found in the Nullarbor, and coral reefs. By understanding how nature engineers complex structures in the environment, we may be able to mimic this to create new materials that have unique properties. We can also learn how to modify the polymer membranes used for desalination to make them repulsive to carbonates to reduce the need for descaling. Furthermore, by developing a full understanding of the growth processes for minerals we may be able to accelerate the design of means to sequester CO2 for long-term storage as carbonates. To date we have already uncovered new details of the early stages of calcium carbonate formation. Here we showed that the initial association of ions is actually favourable (in contrast to expectations from traditional theories) because a dynamic form of inorganic polymer is created in which ions constantly add and detach from solution while the structure of the polymer itself evolves. The discovery of this new mineral precursor is just a first step towards the goal of understanding how minerals can be created and manipulated.

To date, with the assistance of IVEC, ECOCEAN has been able to achieve the following:

40000+ photos collected
21000+ sighting reports
4000+ whale sharks collaboratively tagged
3400+ data contributors (from 53 countries)
365 research days/year

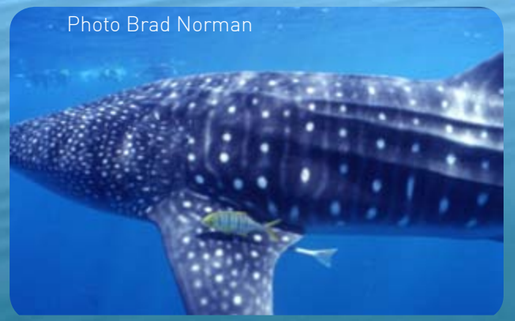


Photo Brad Norman

Photo Brad Norman

Murdoch UNIVERSITY

ECOCEAN WHALE SHARK PHOTO-IDENTIFICATION LIBRARY

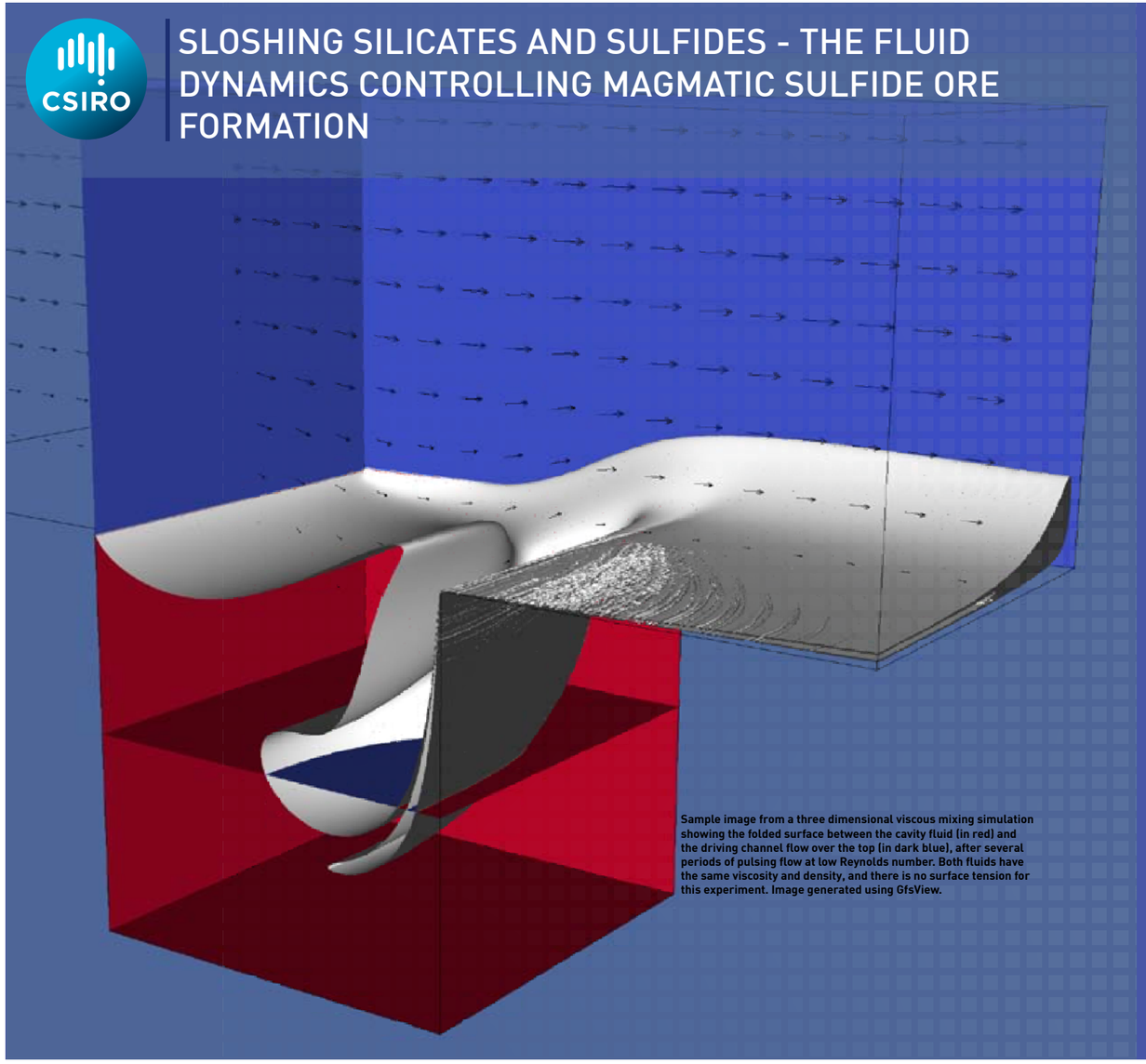
Project leader
Jason Holmberg

Project Overview

The ECOCEAN program has expanded greatly in recent years, with whale shark sighting reports submitted to the ECOCEAN Whale Shark Photo-identification Library from participants in 53 different countries.
To date in 2012, 21000+ sighting reports have been submitted to the ECOCEAN Library. With this significant increase in sighting reports comes a huge increase in scanning requirements to determine whether the same whale sharks are being resighted or whether new previously unidentified sharks are moving to an area.
The WA Department of Environment and Conservation (DEC) utilised images/videos of whale sharks collected by whale shark ecotourism industry operators in 2012 and submitted a total of 1263 encounter reports to the ECOCEAN Library.
The resulting workload would not be possible using traditional methods rather than supercomputing.
IVEC's resources have enabled this project to keep up with the expansion in uptake of the program from citizen scientists (and qualified scientists) worldwide.
It has also enabled the scanning jobs to be completed in a timely manner which further encourages external participants to become (and stay) involved in the wildlife monitoring project (the ECOCEAN Whale Shark Photo-identification Library).

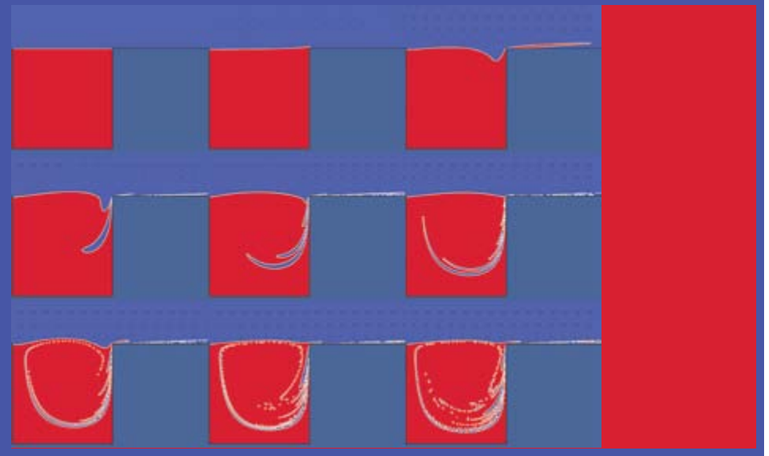
Using IVEC resources to process the sighting encounters submitted by members of the general public has enabled fast feedback to the participants - meaning that we can inform submitters on information concerning 'their' shark i.e. if it has been seen before, where it has been seen before, if it is a new shark etc. This provides the 'citizen scientists' with a sense of ownership and recognition that 'their' submission is being used (and not going into a black hole).

SLOSHING SILICATES AND SULFIDES - THE FLUID DYNAMICS CONTROLLING MAGMATIC SULFIDE ORE FORMATION

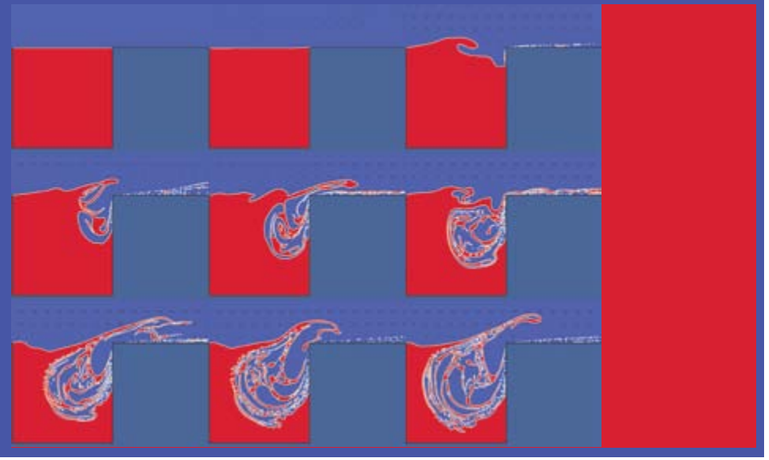


Sample image from a three dimensional viscous mixing simulation showing the folded surface between the cavity fluid (in red) and the driving channel flow over the top (in dark blue), after several periods of pulsing flow at low Reynolds number. Both fluids have the same viscosity and density, and there is no surface tension for this experiment. Image generated using GfsView.

A sequence showing the evolution of mixing between a periodically driven channel flow (blue fluid) and a cavity fluid (red), at moderate Reynolds number (Re=246, based on the driving flow velocity and cavity width as scales). Image generated using GfsView.



A sequence showing the evolution of the mixture in the cavity under the same conditions as Figure 1, except that the cavity fluid is now denser and less viscous than the overlying driving flow. Image generated using GfsView.



Project leader

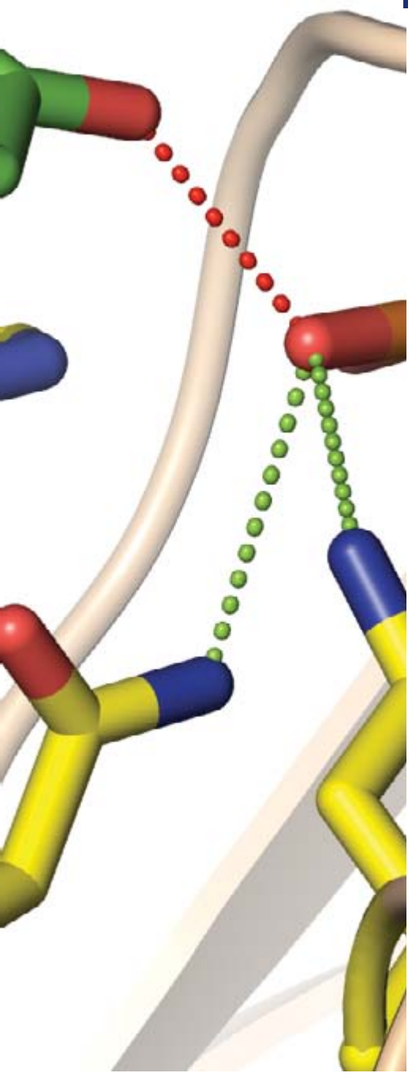
Jess Robertson

Project Overview

Magmatic sulphide ore deposits supply the majority of the world's nickel reserves, and almost all of the world's platinum. This project deals directly with the fundamental physical process key to their formation: the entrainment, transport and deposition of immiscible sulphide liquid within silicate magma. This is a fundamental problem whose solutions are key to the design of exploration programs looking for new deposits, and also for understanding the mine-scale geometry and internal structure of orebodies. However, the fundamentally three-dimensional nature of these processes puts the numerical studies of these flows firmly out of the reach of desktop computing. iVEC supercomputing resources, expertise and implementation of Gerris (a massively parallel adaptive fluid dynamics code - see http://gfs.sourceforge.net) has allowed our team to unravel the complex interactions between sulfide and silicate magmas.

UNIVERSITY OF TECHNOLOGY SYDNEY

ALLOSTERIC CONTROL OF ATP HYDROLYSIS IN THE ABC TRANSPORTER CATALYTIC CYCLE



Project leader

Peter M Jones

Project Overview

ABC transporters comprise a biomedically important superfamily of enzyme "pumps", that move compounds across the membrane that encloses all living cells. Some ABC transporters mediate multidrug resistance (MDR), exhibited by many cancers and pathogenic microbes, where drugs are pumped out of the cell, thereby nullifying their effect. Understanding the ABC transporter molecular mechanism is required for the development of new therapies to circumvent MDR. Molecular Dynamics (MD) Simulation is a computational technique made possible by modern high performance computers, and is powerful in its unique ablility to reveal dynamic aspects of a protein's mechanism. We used MD analysis of the "engine" domain of the ABC transporter pump, which comprises two identical subunits, that bind two small "fuel" molecules (ATP) in two "active sites" formed at their interface. Controversy surrounds whether the motor subunit pair, or dimer, disengages completely (Switch Model) or not (Constant Contact Model). According to the Switch Model, the state simulated should have resulted in complete separation of the motor subunits, but according to the Constant Contact Model, only the one site should open. We observed the latter, thus resolving the issue. Importantly, our analysis additionally revealed how the active site opens by way of internal subdomain rotations.

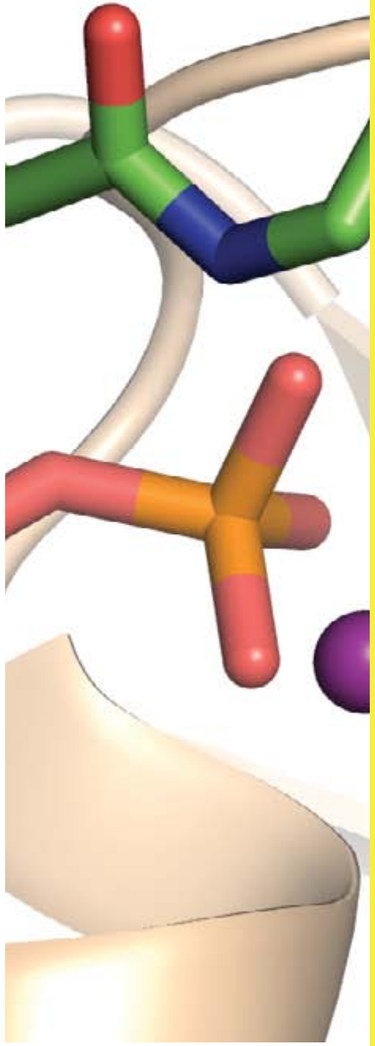


Figura 1. Structure of the ADP+Pi-bound ABC Dimer. Cartoon representation of the ABC transporter motor domain dimer used as the starting structure for the MD simulations. Separate subunits are situated top and bottom; principal subdomains coloured "wheat" and "slate". ADP+Pi molecules, the product of ATP breakdown, are bound at the intermonomer interface, and shown in stick representation, with carbon yellow, oxygen red, nitrogen blue, and phosphorous orange. Catalytic metal is shown as a purple sphere.

Figura 2. Opening of the empty active site via relative movements of core and helical subdomains. View of the MD trajectory frame corresponding to the maximum opening of the empty active site, showing rotating domains and their hinge axes. Axes are longer red, blue and green lines, with the two shorter same-coloured lines connecting the centre of mass of the rotating domain to the pivot point on the axis. Cartoon image of the protein with monomer A bottom and monomer B top. Rotating core subdomain of monomer B is coloured cyan and its hinge axis is in red. Rotating helical subdomain of monomer B is coloured magenta and its hinge axis is in green. Rotating helical subdomain of monomer A is coloured orange and its hinge axis is in blue.

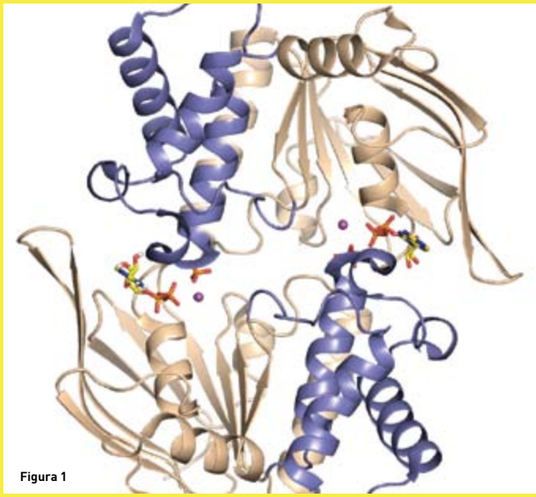


Figura 1

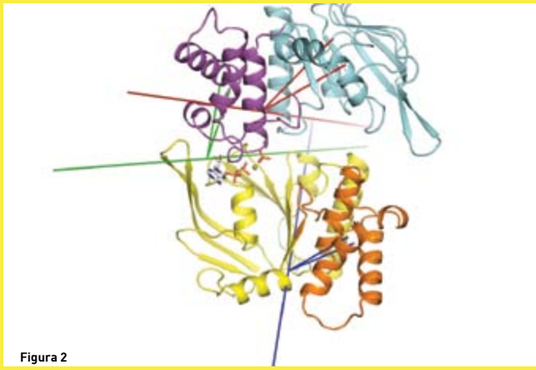
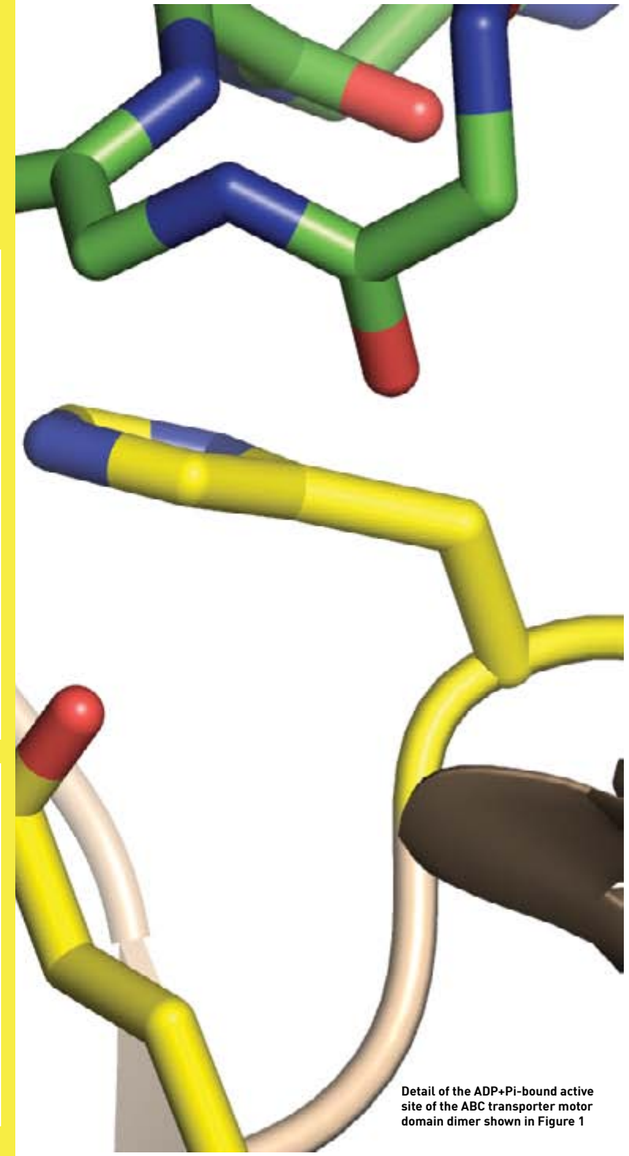


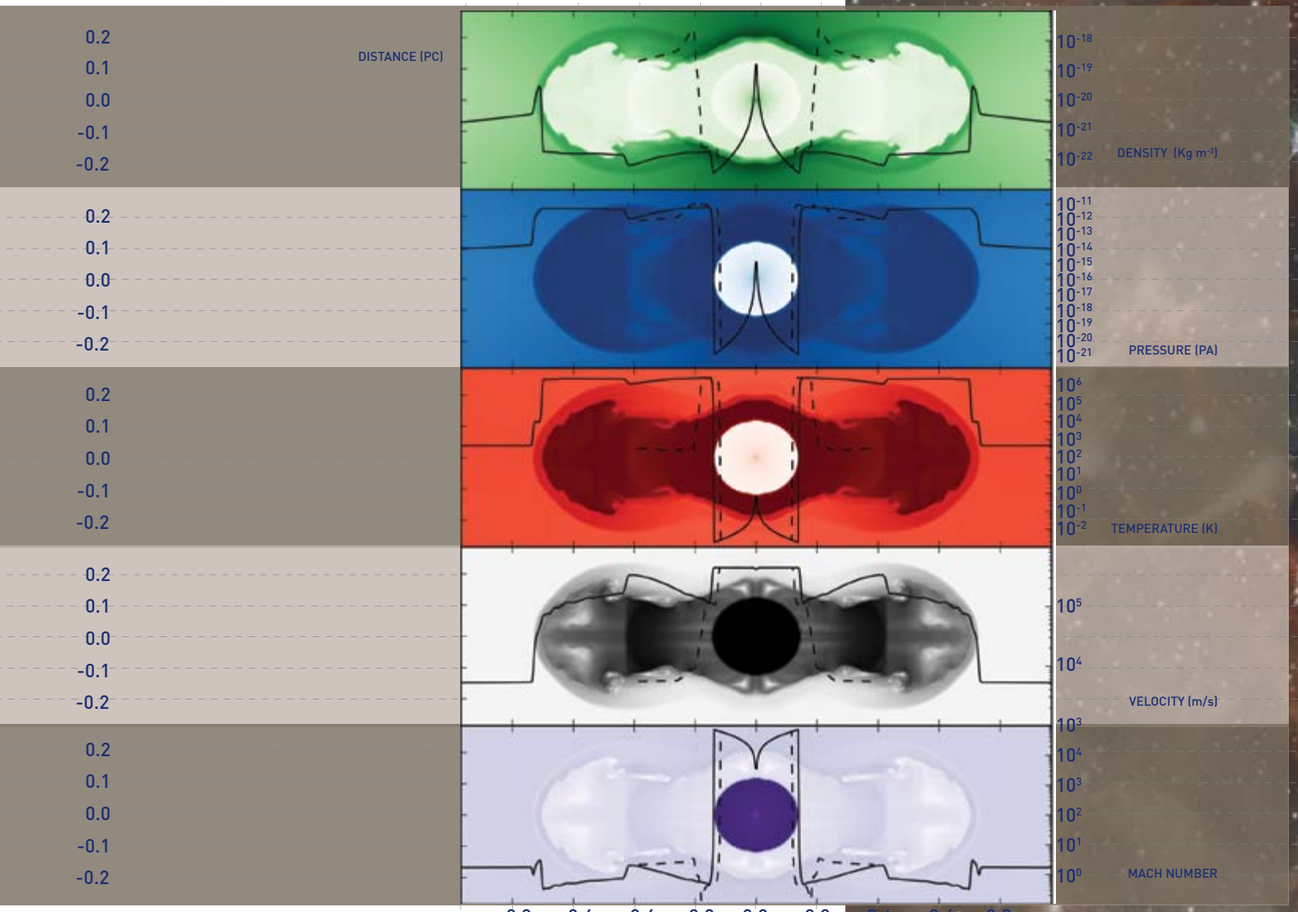
Figura 2



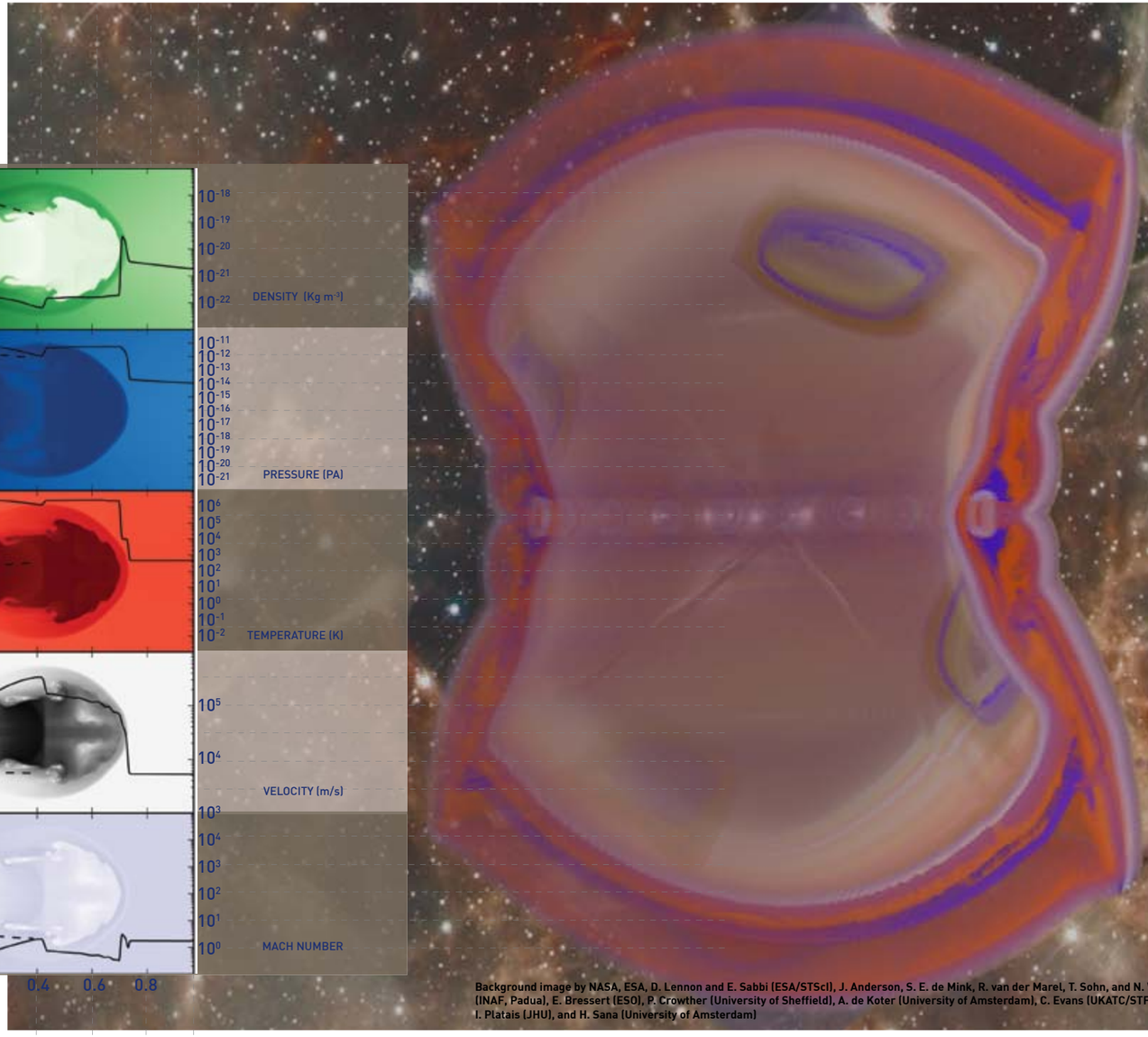
Detail of the ADP+Pi-bound active site of the ABC transporter motor domain dimer shown in Figure 1

International Centre for Radio Astronomy Research

MULTIDIMENSIONAL SIMULATIONS OF THE EXPANDING SUPERNOVA REMNANT SNR 1987A



In this plot is the final set of plots of a simulation to model the formation of the pre-supernova environment of SN1987A.



Background image by NASA, ESA, D. Lennon and E. Sabbi (ESA/STScI), J. Anderson, S. E. de Mink, R. van der Marel, T. Sohn, and N. Walborn (STScI), N. Bastian (Excellence Cluster, Munich), L. Bedin (INAF, Padua), E. Bressert (ESO), P. Crowther (University of Sheffield), A. de Koter (University of Amsterdam), C. Evans (UKATC/STFC, Edinburgh), A. Herrero (IAC, Tenerife), N. Langer (AifA, Bonn), I. Platais (JHU), and H. Sana (University of Amsterdam)

Project leader

Toby Potter and Lister Staveley-Smith

Project Overview

In this project we combine high performance computing with semi-analytic models to model radio emission from the well known supernova remnant SNR 1987A. This allows us to gain insight into the physics of particle acceleration at supernovae shocks.

Our approach is to simulate the expansion of the remnant in three dimensions using a parallel fluid dynamics research code. In order to simulate the explosion with sufficient resolution we needed to use compute resources exceeding the capacity of most desktop computers.

As a result of this investigation we have been able to place an empirical estimate on the efficiency of particle acceleration at astrophysical shocks.

This potentially has direct relevance to the SKA project because it will allow us to predict the level of radio emission from the cosmic web.

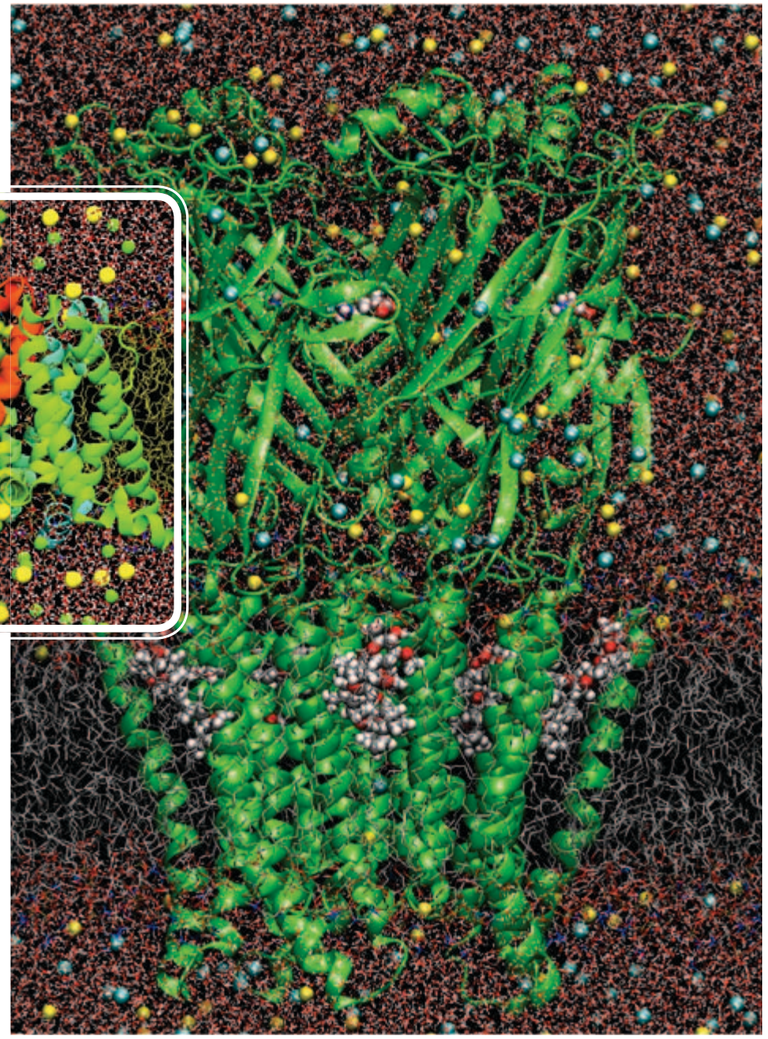
Shown is a render of the final model from the simulation as it might appear in 2014. Orange is the log of radio emission; purple is log X-ray; and tan and white is the log of entropy, which highlights the shocks. The structure is about 3 light years in diameter.

RMIT UNIVERSITY

MECHANISMS OF CHARGE-MEMBRANE INTERACTIONS AND TRANSPORT

Project leader

Assoc. Prof. Toby W. Allen



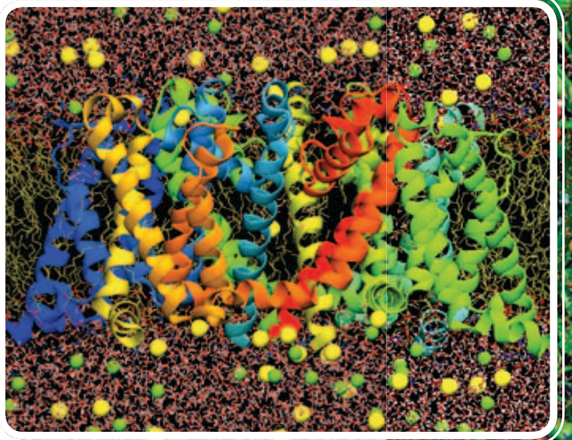


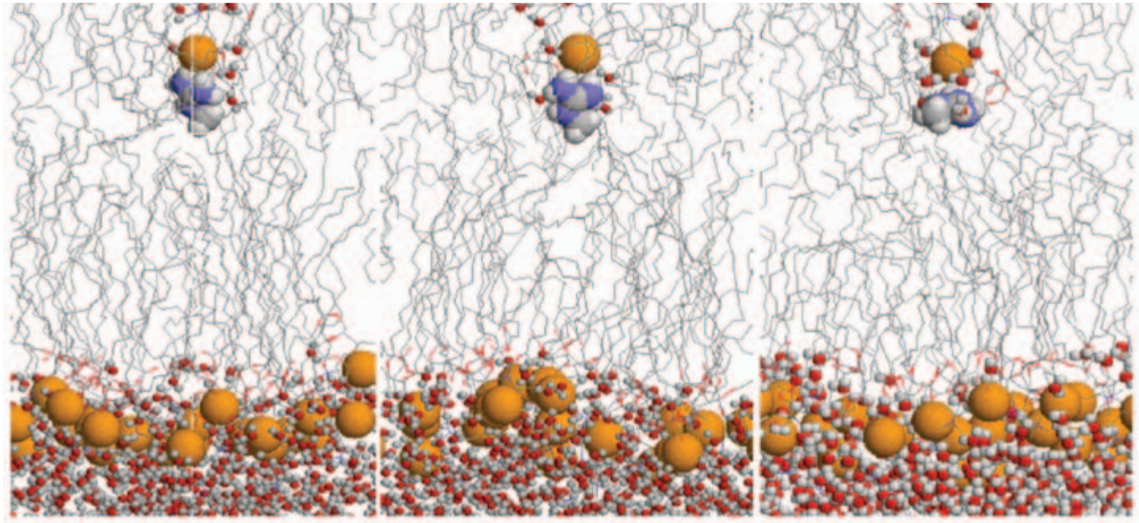
Fig.2. Voltage-gated sodium channel (coloured ribbons) embedded in a lipid membrane (yellow chains) solvated by electrolyte solution (water – small red/white sticks, Na+ and Cl- ions as green and yellow balls).

Fig.3. Pentameric ligand-gated ion channel, GluCl, from roundworm, showing the protein (green), with bound glutamate agonists (extracellular domain – upper; space-fill CPK representation) and anti-parasitic drug ivermectin (trans-membrane domain – lower; space-fill CPK representation) holding channel open, sitting in a lipid bilayer membrane (grey chains) solvated by electrolyte solution (water – small red/white sticks, Na+ and Cl- ions as cyan and yellow balls).

Project Overview

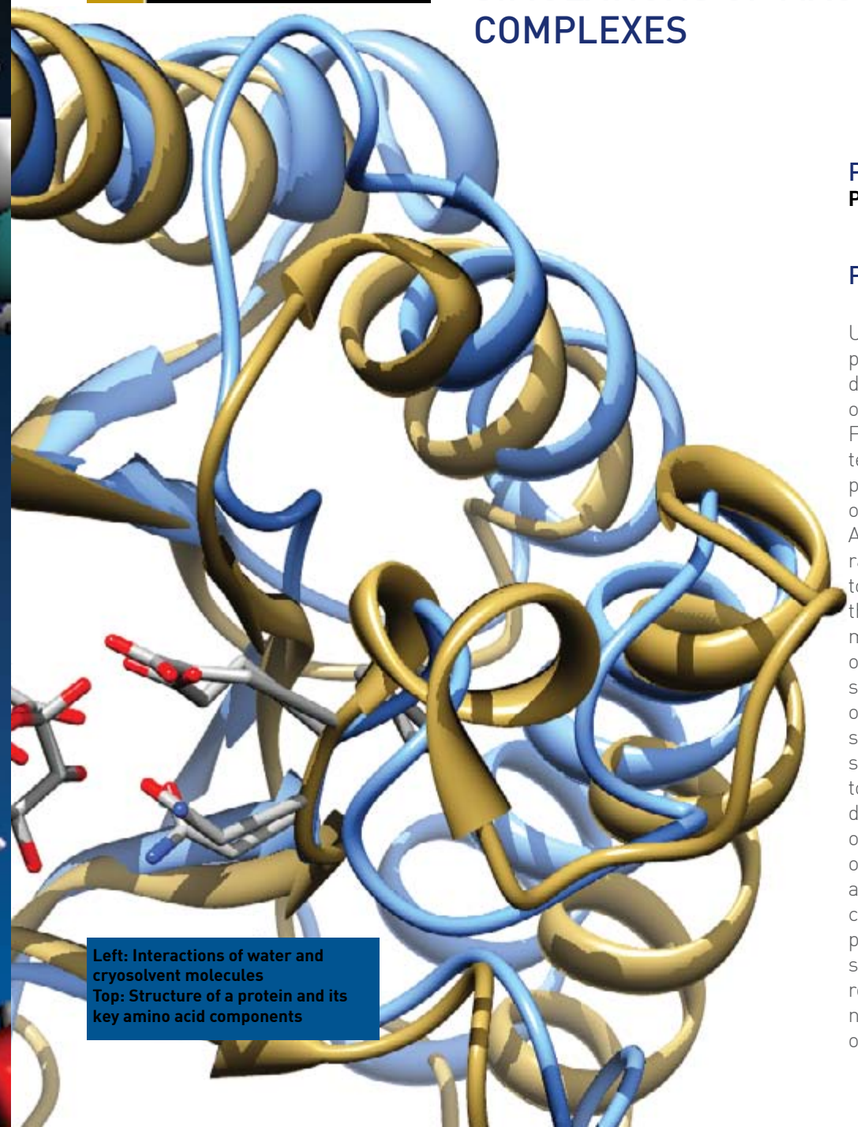
Membranes mediate biological activity by providing gateways into cells and homes to a range of proteins with critical functions. This research aims to uncover the physical and chemical rules underlying membrane charge transport using atomic-level simulations that reveal how membrane composition can modulate the transport of ions, as well as the actions of cell-perturbing viral, toxin and antimicrobial peptides. It also explores the mechanisms of channel-mediated ion movement across membranes and the role of membrane chemistry in function. These studies will improve knowledge of biological membranes for the future developments of novel therapeutics and bionanodevices for medical research. This work also improves understanding of the actions of cell-perturbing peptides responsible for the delivery of cargoes across biological membranes. Elucidating these mechanisms, as well as their specificity for particular cell membranes, is the first necessary step for understanding infectious disease, antimicrobial activity, the actions of toxins and potential therapeutic capabilities, and for the design of drug or gene delivery and nano-biosensing applications. This work addresses important problems that will impact on several ARC priority areas, including: breakthrough science in the form of state of the art computational methodologies for biological systems; in advanced materials, through a higher level of understanding for the development of peptides that can deliver biosensing nanodevices or drugs to cells, with future medical advances for promoting and maintaining good health.

Fig.1. Monounsaturated lipid bilayers (24 carbon case shown here) thickened by cholesterol reveal membrane deformations to stabilise an arginine analogue molecule, even at the centre of the membrane. Three independent samples shown. Arginine is shown in CPK space-fill representation, lipid membrane as grey chains and orange phosphate P atoms (seen to have moved into the membrane to coordinate the ion), and water as small red/white sticks. Simulations as a function of chain length and cholesterol content reveal free energy barrier height increasing dramatically (not shown).



Curtin University

LARGE SCALE MOLECULAR DYNAMICS SIMULATIONS OF MACROBIOMOLECULAR COMPLEXES



Left: Interactions of water and cryosolvent molecules
Top: Structure of a protein and its key amino acid components

Project leader

Prof. Ricardo L. Mancera

Project Overview

Understanding complex biological phenomena is essential for the development of drug molecules and/or novel biotechnological approaches. For example, understanding the tendency for aggregation of certain proteins that leads to the formation of fibrilles and the development of Alzheimer's disease is essential for the rational design of new drug molecules to cure this disease. Characterising the extent of damage suffered by cell membranes under physical stress is of crucial importance for developing successful cryopreservation protocols of plant material of endangered species. Molecular dynamics computer simulation methods are ideally poised to investigate these phenomena in great detail, requiring however large numbers of compute nodes for large periods of time in order to access the length and timescales required to investigate complex biological processes. High-performance computing and data storage facilities thus provide excellent resources to tackle systems that would not be possible to investigate in any other way.

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RANDOM SPACE FILLING

Project leader
Paul Bourke

Project Overview

Many physical processes involve a packing of objects into a region of space, with examples being found in materials science and geoscience. Traditionally, simulated models of these processes involve randomly adding objects into available gaps and growing them until they touch another pre-existing object. These are so called Apollonian packings where neighbouring objects touch (kiss) each other, despite the fact that many physical processes don't appear to exhibit that phenomena. The model explored here asks the question "How does one iteratively place objects randomly into a region using a monotonically decreasing function for the area of the object such that the space is filled?". On each iteration, if the area of the next shape to be added decreases to quickly then the space will not be filled. If the area decreases too slowly one ends up in a situation where there is no free gap large enough to place the next object and the algorithm cannot continue. The solution studied and simulated here turned out to be very elegant and general, and in some ways surprising. The special function of area is such that it can be applied to the packing any object shape and into any arbitrary shaped region. For this project the simulations have been performed in 1, 2 and 3 dimensions. The resulting packing is fractal in the sense that as one zooms in, the appearance is self similar and further, the fractal dimension can be controlled suggesting that it may be a model for a range of natural phenomena.

Figure 1: Filling a rectangular region with torii, an example of the independence of the filling shape.

Figure 2: Filling a toroidal shape with rectangles, illustrates the independence of the area to be filled.

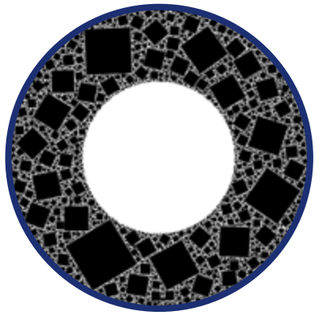
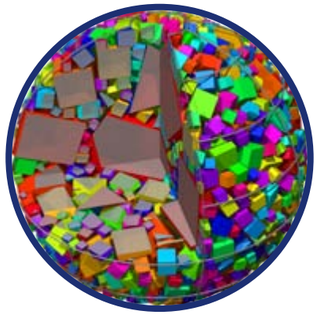
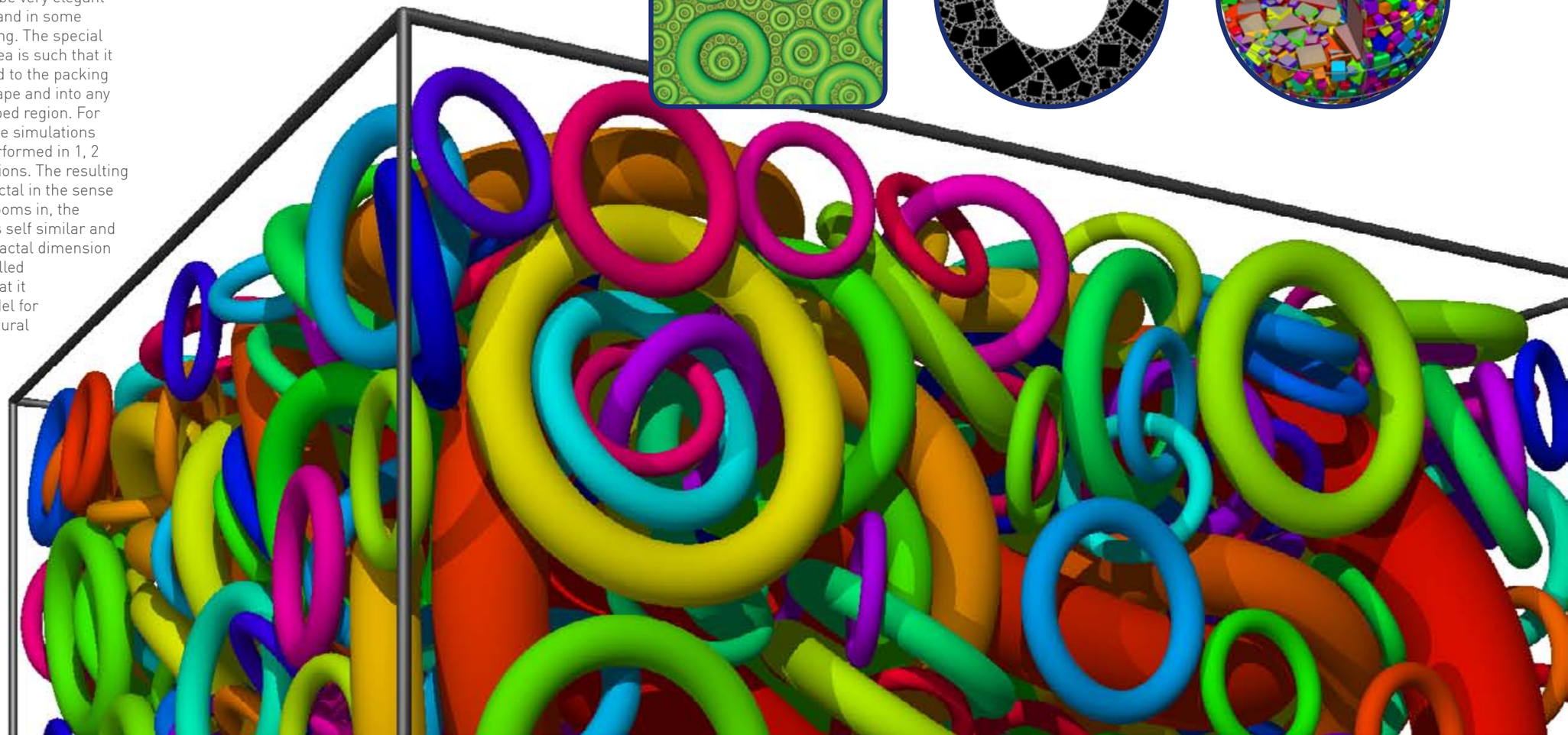


Figure 3: Cut-away section showing cubes filling a sphere.





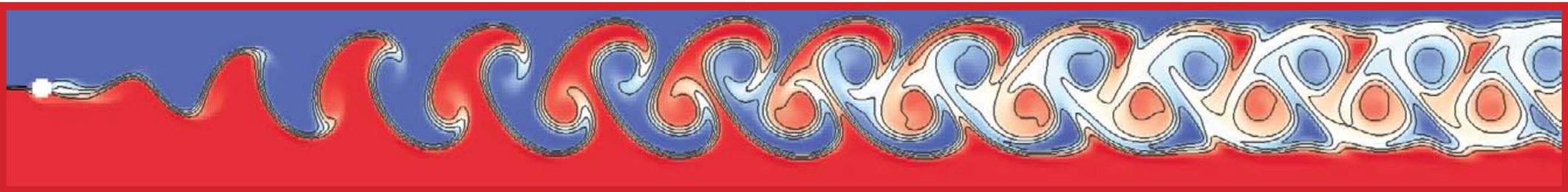
GEOSCIENCES START-UP PROJECT

Project leader
Terry Rankine

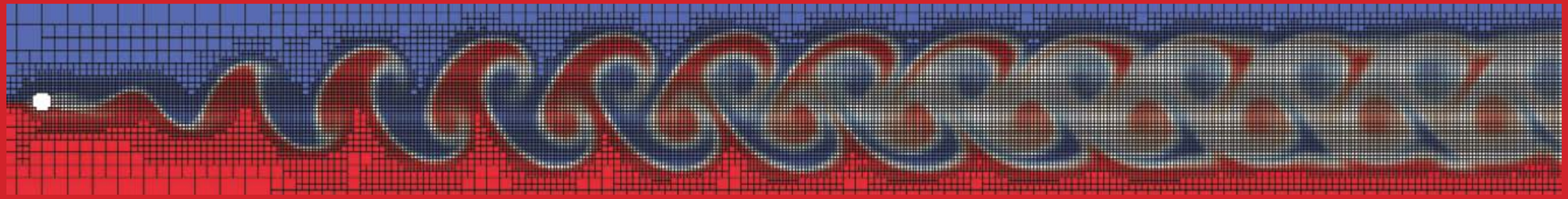
Geoscientists working in research areas involving numerical simulations tend to spend a lot of their time experimenting with numerical codes to suit their need. Ideally, these scientists try to choose codes which will enable them to scale their simulations to large systems using computer clusters once a working model has been implemented, but the time needed to get to that point is often hard to predict in advance. As a result, it is often difficult for them to anticipate how many resources will be required at the time.

The purpose of this project was to allow some CSIRO geoscientists to have access to iVEC's infrastructure through a "group allocation". This project played its role effectively as users were provided access to Epic@Murdoch through this scheme when they needed access at any point during the year, without having to make a formal request.

Several people in the group enjoyed this opportunity, including Dr Jess Robertson, who investigated several different codes on iVEC infrastructure, especially Gerris (http://gfs.sourceforge.net), a self-adaptive, massively parallel fluid dynamics package. The iVEC team and the Epic@Murdoch supercomputer allowed us to benchmark this code at a much larger scale than was previously possible.



Cylinder benchmark simulating a von Karman street of vortices with diffusing tracer behind a cylinder in moderate-Reynolds number flow. This is a small benchmark used to test Gerris on Epic for small to moderate numbers of processors.



Cylinder benchmark showing dynamically adapted semi-structured grid.

Spatial decomposition across 16 processors for the cylinder benchmark . All the images generated using GfsView'

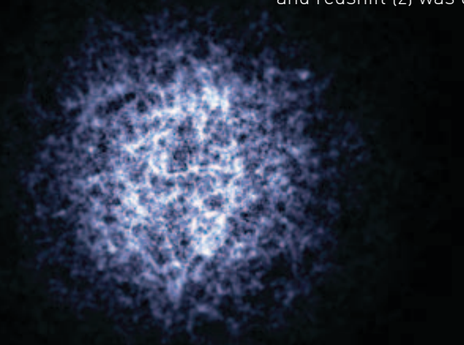
International Centre for Radio Astronomy Research

ASKAP SIMULATIONS
EXPLORING THE SIMULATED GALAXY CATALOGUES FOR THE ASKAP NEUTRAL HYDROGEN SURVEYS

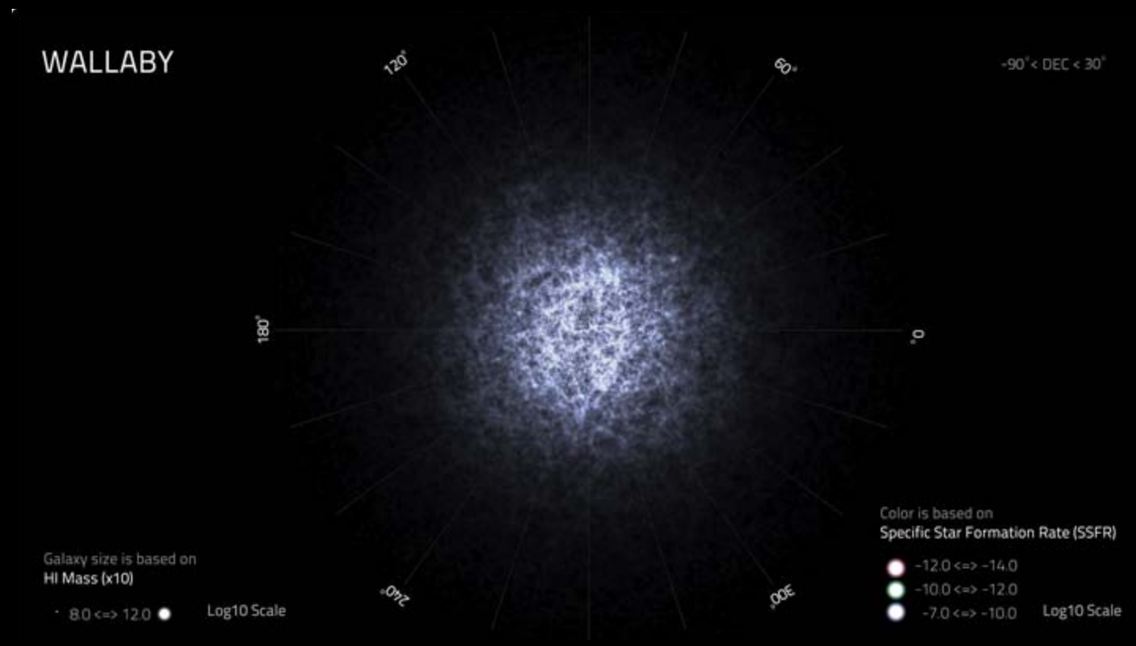
Project Team Dr. Alan Duffy & Derek Gerstmann

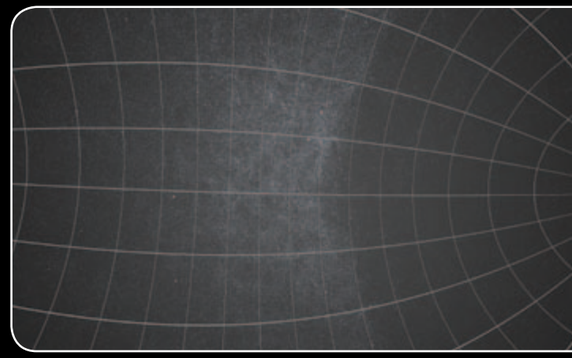
Project Overview

The Australian Square Kilometre Array Pathfinder (ASKAP) will revolutionise our knowledge of gas-rich galaxies in the Universe. In this video, we focus on visualising the galaxy catalogues created for two proposed extragalactic ASKAP neutral hydrogen (HI) surveys, based on semi-analytic models applied to cosmological N-body simulations (Duffy, et al 2012 *). These surveys will find 40 times more galaxies, across 1000s of times more of the Universe, than any HI survey before; demanding cutting edge simulations to create the predictions as well as visualise them. Two survey projects are revealed in the video -- the first, known as WALLABY, or the ASKAP HI All-Sky Survey, is a shallow all-sky survey which will probe the mass and dynamics of over 600,000 galaxies. The second survey project, DINGO (overlayed and revealed in the later portion of the video), is a much deeper, smaller-area HI survey, aiming to trace the evolution of HI in potentially 100,000 galaxies across the last 4 billion years of cosmic time.
The frames in the video were created by an interactive motion-compensated, point-based rendering system developed at ICRAR, called Gaius, which has been designed specifically for large scale astronomy and astrophysical datasets. For this video, the spatial coordinates in the catalogue were converted from right-ascension (RA) and declination (DEC) to direction cosines across the sky, and redshift (z) was used to provide a distance from the point of observation. In this case, the centre represents the location of the observer (the earth, or more specifically, the site of the ASKAP telescope at The Murchison Radio-Astronomy Observatory (MRO) in rural Western Australia). Each point corresponds to one galaxy in the catalogue -- HI mass has been used to weight the elliptical radius of each point, and the colour corresponds to the observed colour range for the type of galaxy, based on its predicted star formation rate. Every galaxy from the simulated catalogues is shown. Each frame from the interactive renderer was saved to disk at 2k resolution as 32-bit floating point OpenEXR files, before being encoded to ProRes using Apple's Compressor. Titles and editing were done in Apple's FinalCut Pro X.



Predictions for ASKAP Neutral Hydrogen Surveys (accepted to MNRAS)
* http://arxiv.org/abs/1208.5592

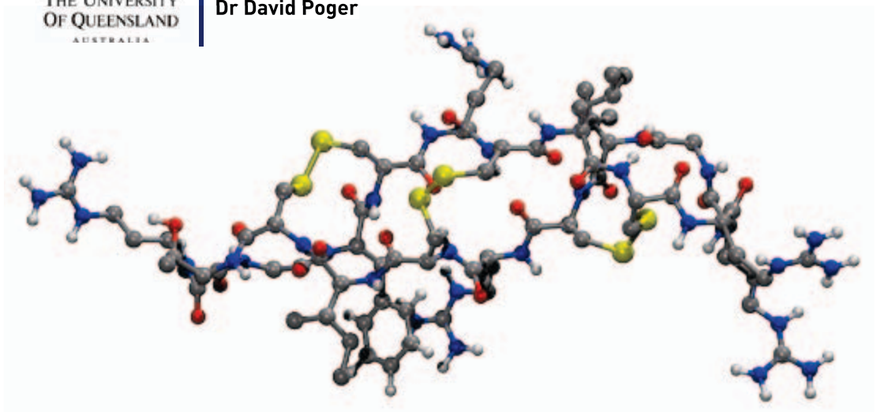




PROTEIN SELF-ASSEMBLIES AT MEMBRANE INTERFACES

Project leader

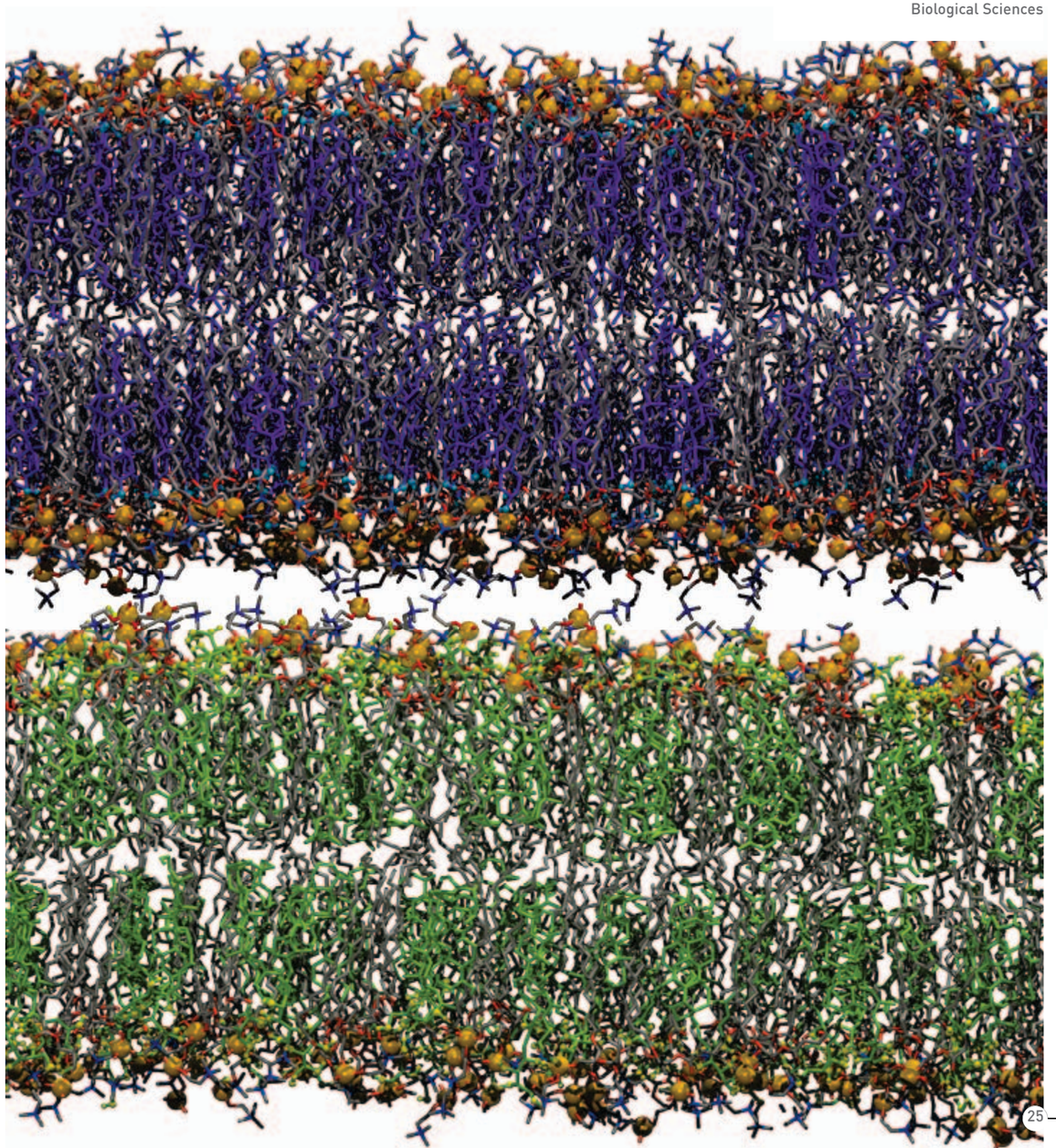
Dr David Poger



LEFT; Structure of the antimicrobial peptide RTD1 after 200 ns of simulation in water

Project Overview

How biomolecules interact and self-assemble in a membrane context is one of the grand challenges of modern biology. The structure and dynamics of biological membranes, membrane proteins (such as the receptors for erythropoietin and growth hormone) and membrane-active molecules (such as antimicrobial peptides and natural antioxidants), is at the forefront of research in structural biology. Although essential, only now are lipids being considered as important modulators and determinants of selectivity and specificity for the binding of molecules on to membranes and the development of new antibiotics. It is all the more critical that the membrane composition differs between organisms, cell types and organelles and varies over the course of the cell cycle. To carry out this project, the behaviour of molecules—specifically the movements of the tens to hundreds of thousands of atoms that make up lipids and proteins—are modelled as a function time. Atomistic simulations of large systems like biological membranes and protein–membrane systems are computationally expensive and require extensive calculations that can only be performed on state-of-the-art facilities such as Epic at iVEC. The resulting trajectory (basically a movie) can be used to evaluate structural and functional properties of membranes and membrane-binding molecules.



Structure of a lipid bilayer containing an equimolar mixture of 2-oleoyl-1-palmitoyl-*sn*-glycero-3-phosphocholine (POPC) and cholesterol (the polycyclic backbone is displayed as purple sticks and the headgroup as cyan spheres). The phosphorus atom in POPC is shown as an orange sphere. The structure was obtained after 400 ns of simulation.

Structure of a lipid bilayer containing an equimolar mixture of 2-oleoyl-1-palmitoyl-*sn*-glycero-3-phosphocholine (POPC) and the biohopanoid bacteriohopanetetrol (the polycyclic backbone is displayed as green sticks and the headgroup as yellow spheres). The phosphorus atom in POPC is shown as an orange sphere. The structure was obtained after 450 ns of simulation.

Acknowledgements

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Australian Government