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Modelling and Simulation

Hans Fangohr
Professor of Computational Modelling

Computational Modelling

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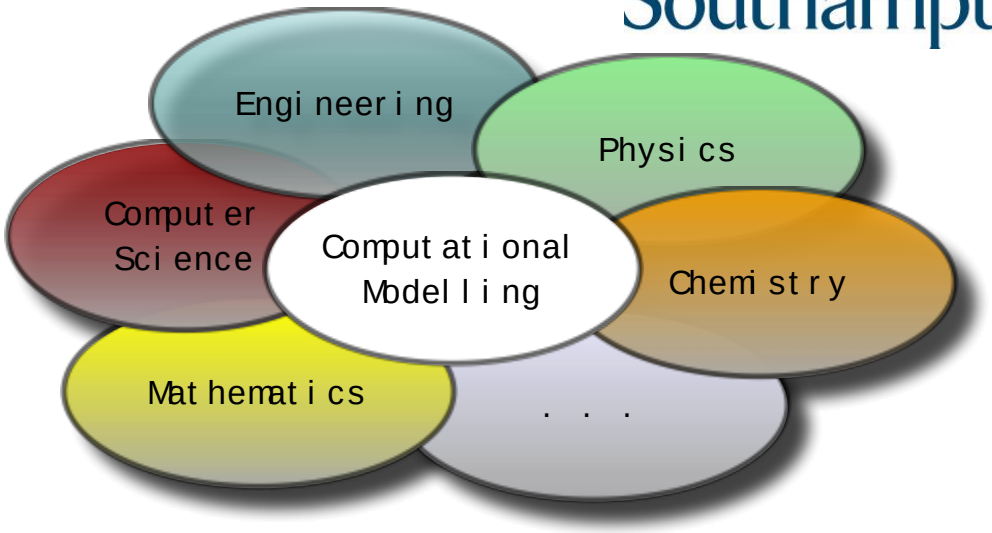

- Computational Modelling plays key role in research and development
- Significant underpinning technology at Southampton
  - *Computational Modelling Group* (cmg.soton.ac.uk)
  - Interdisciplinary training and research

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Computing @ University of Southampton

Pegasus (1950's)

ICL (1960's & 70's)

IBM3090 (1980's)

IBM SP2 (1990's)

Iridis1-4 (2001-2013)

Mission

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- to *apply computational modelling* to advance science and engineering in academia and industry
- to *research computational methodology* to enable and advance most effective computational modelling for the present and future

Simulation across the domains

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Physical Systems and Engineering simulation

Acoustics (12), Advanced Materials (5), Astrophysics (10), Biomechanics (13), Biometrics (2), Catalysis (2), CFD (58), Climate (14), Combustion (4), Complex fluids (10), Data Acquisition (5), Diffusion (9), Earth Observation (8), Earth surface dynamics (14), Elasticity (6), Electromagnetism (17), Energy (20), Fiber Optic Communications (4), Flight simulation (5), Flow Control (1), fluid structure interaction (9), Free surface flows (3), General Relativity (5), Geophysics (4), Heat transfer (10), Hydrology (3), Landscape evolution (6), Liquid crystals (2), Magnetohydrodynamics (2), Magnonics (7), Marine Renewable Energy (5), Materials (30), MEMS (3), Metals (6), Micromagnetics (19), Oceanography (11), Particle Collisions (3), Photonics (15), QCD (7), Quantum Dynamics (5), Robotics (1), Sediment transport (9), Semiconductors (8), Sensors (6), Sexual Health (1), Ship Hydrodynamics (4), Spintronics (4), Structural dynamics (12), Superconductivity (4), Superfluidity (1), Thin film flow (1), Tribology (6), Turbulence (24), Wave propagation (10), Wireless Communications (3)

Socio-technological System simulation

Air-traffic Control (1), Archaeology (5), Built Environment (3), Economic Networks (6), Healthcare modelling (3), Human environment interaction (13), Human population (12), Operations Research (4), Self Organized Networks (6), Sensor Networks (3), Social and Socio-economic Systems (18), Social Networks (17), Transport (8), Value-driven design (4)

Life sciences simulation

Bioinformatics (34), Biomathematics (12), Biomedical (31), Biomolecular Organisation (8), Biomolecular simulations (21), Developmental Biology (4), Ecology (25), Environmental hazards (5), Epidemiology (6), Epigenetics (3), Evolution (18), Medical Imaging (2), Microbiology (1), Nanoscale Assemblies (4), Neuroscience (9), NextGen Sequencing (14), Psychology (2), Structural biology (7), Swarm Behaviour (6), Systems biology (18), Tissue Engineering (3)

Wide range of methods & tools

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Algorithms and computational methods

Agent-Based Negotiation (2), Agents (47), Artificial Neural Networks (8), Boundary elements (6), Cellular automata (14), Classification (7), Computer Vision (1), Density functional Theory (14), Distributed computing (6), Evolutionary Algorithms (13), FFT (25), Finite differences (46), Finite elements (34), Finite volume (20), Game Theory (10), Geographic Information Systems (11), Graph Theory (5), Inverse problems (5), Lattice Field Theory (7), Machine learning (7), Maximum Likelihood (1), Meshless methods (3), Minimum Energy Paths (2), Molecular Dynamics (24), Molecular Mechanics (9), Monte Carlo (39), Multi-core (19), Multi-physics (28), Multi-scale (25), Multigrid solvers (7), Multipole methods (2), Optimisation (27), Quantum Chemistry (11), Quantum Computation (4), Smoothed Particle Hydrodynamics (1), statistical analysis (18), Stochastic Pi Calculus (1), Support Vector Machine (3), Symbolic calculation (2)

Visualisation and data handling software

3ds Max (1), Amira (2), ArcGIS (12), Avizo (6), Blender (1), ECCE (1), ENVI (6), Gnuplot (23), h5py (2), HDF5 (13), IDL (5), ImageJ/Fiji (4), Jung (2), Labview (1), Mayavi (12), MS Office Access (4), MySQL (4), NetworkX (1), ParaView (24), PostGres (1), Povray (2), Pylab (22), PyTables (3), Simpleware (2), SQL Azure (1), TecPlot (17), VG Studio Max (1), Virtual Earth (1), VisIt (7), Visual Python (5), VMD (14), VTK (17), Xmgrace (19)

Programming languages and libraries

AWK (2), Boost (1), C (61), C# (5), C++ (60), Chroma (4), CUDA (4), CUDA Fortran (1), Fortran (61), GPU-libs (3), GSL (6), IPython/Jupyter Notebook (11), Java (26), Julia (3), Maple (4), Mathematica (12), Matlab (64), MPI (44), OCaml (4), Octave (1), OpenACC (1), OpenCL (2), OpenMP (22), Perl (6), PETSc (6), Python (96), R (37), Stata (1), Tcl (3), UKHadron (4), Verilog (1), VHDL (1)

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Facilities

Computational Resources

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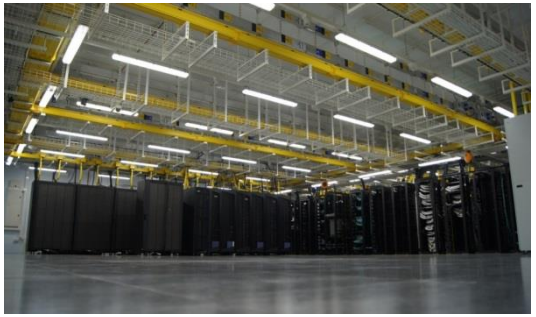
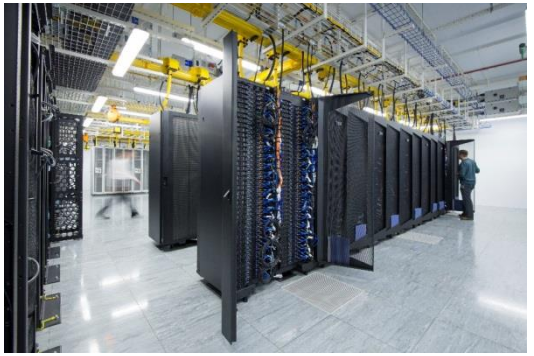
- HPC Cluster at Southampton:
  Linux cluster with 12,200 Cores (250 TFlops), 1.04 PB of disk storage
  largest University super computer in England
- Access to ARCHER (UK national HPC system)
  Currently: 72,192 cores, 7.8 Pb memory, 1.56 Pflops
- Specialised and accelerator hardware including Intel Xeon Phi, GPUs, Power8, ARM, FPGA
- large big data shared-memory machines with 96 cores and 2TB RAM each





Iridis 4

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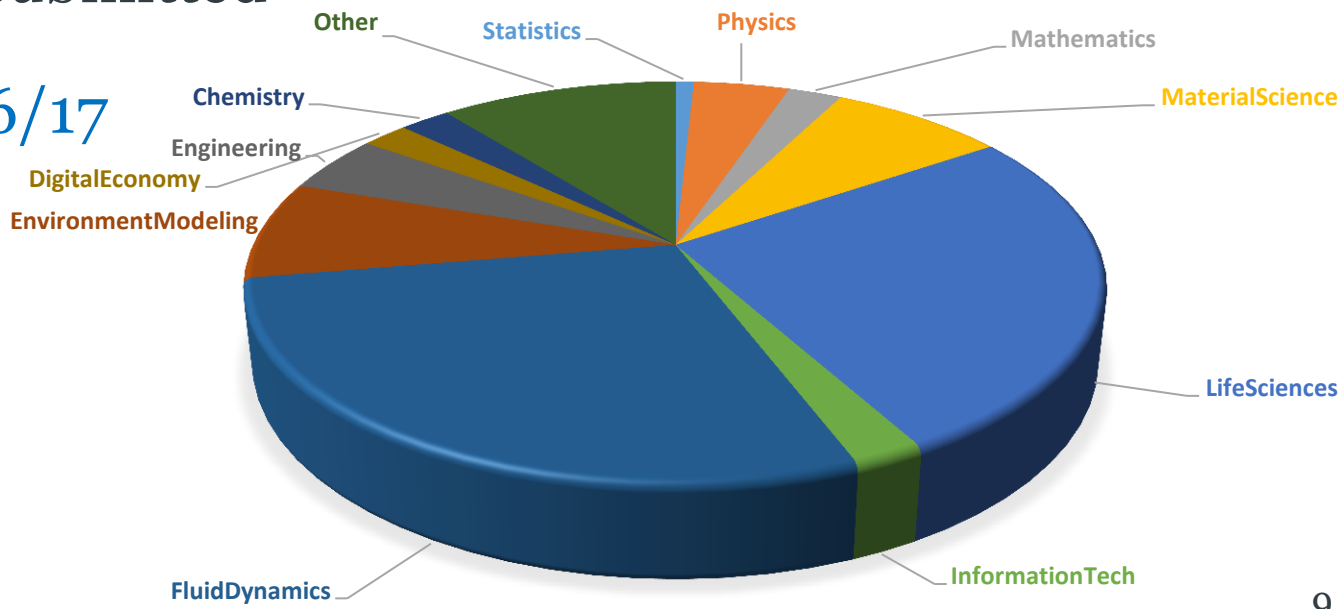
- 1067 registered users
- 437 PI's with registered projects *(>47% UoS Research Income)*
- Projects are from all 8 faculties
- ~2.5M jobs submitted
- Refresh 2016/17



Rolls-Royce

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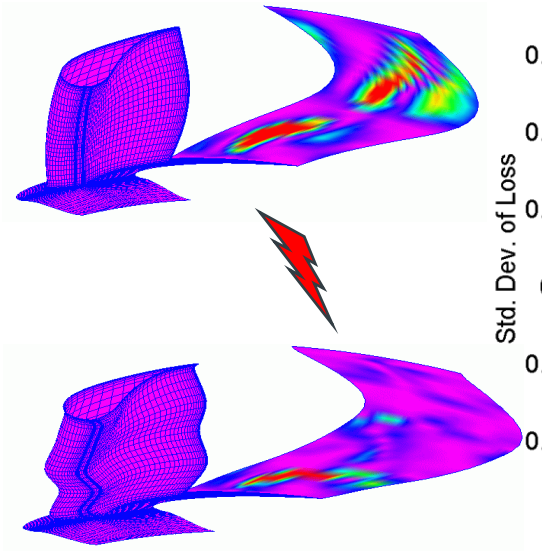
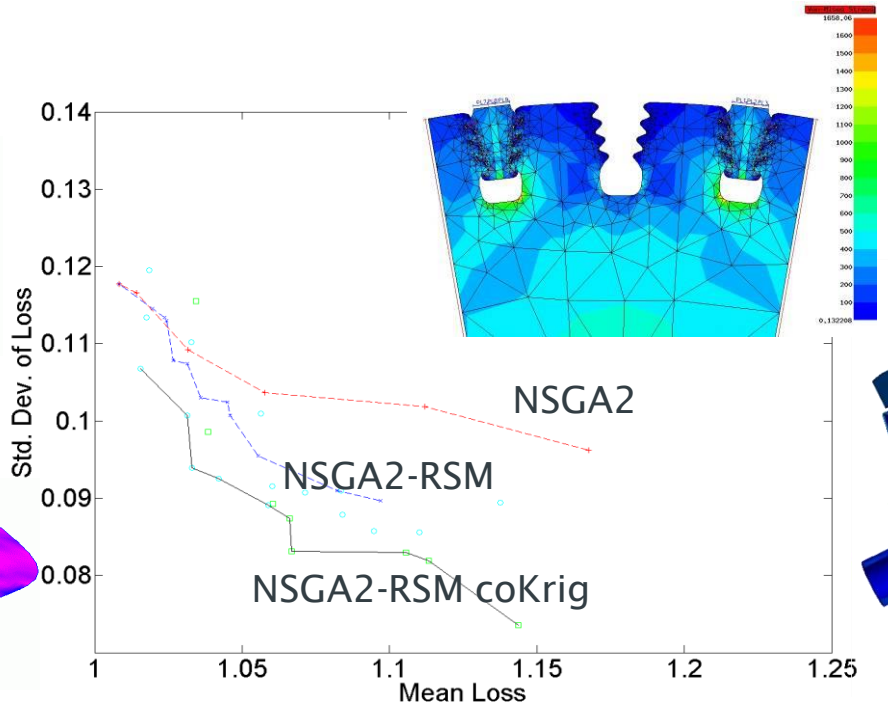
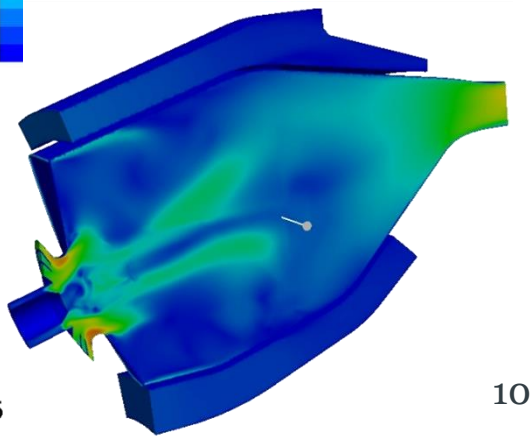
Rolls-Royce UTC in Computational Engineering

PIs: **Keane & Scanlan**

- 3 Academic staff, 6 Research fellows, 7 EngD/PhDs,
- £0.75m per annum external funding (EU/UK Govt/EPSRC)
- Design Optimization, Robustness, Cost Models, Geometry Control
- Close integration with Rolls-Royce R&T objectives







Airbus Noise Technology Centre

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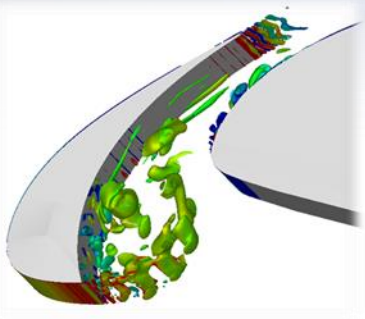
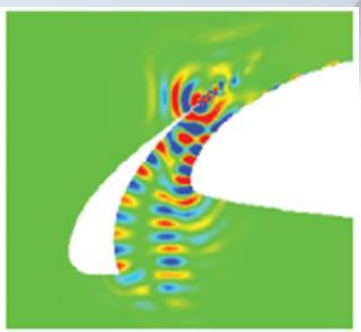
PI: **Angland**

- First Airbus-University Technology Centre in the World
- Opened November 2008
- Focussing on future aircraft technologies for noise reduction
- Fifteen academic staff and research students
- Computation and experiment





UK Turbulence Consortium

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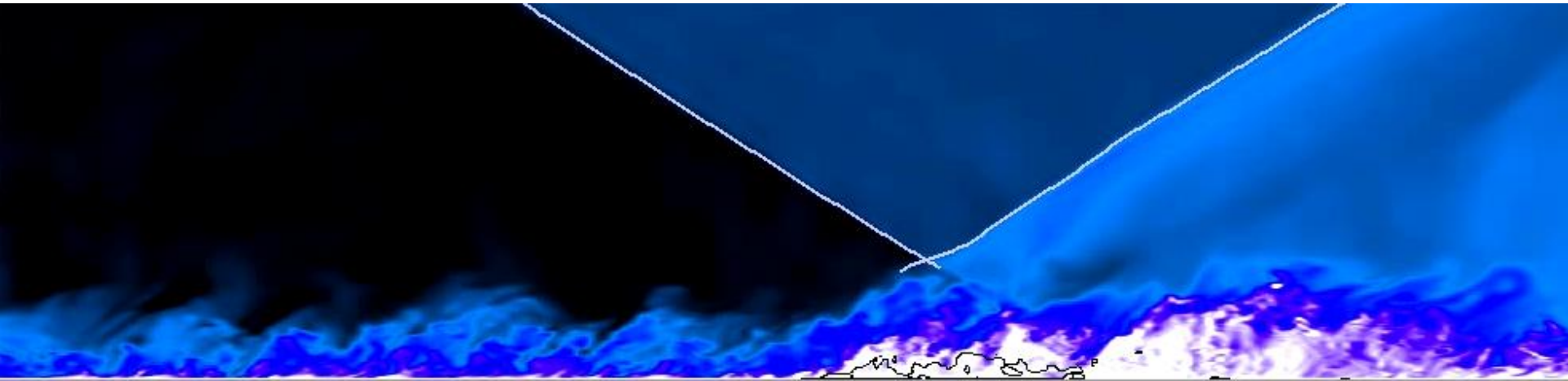
- Managed from Southampton since 1999
- 28 academics at 15 UK institutions
- ***Numerical experiments*** answer *basic questions* regarding physics and modelling of turbulent flows found in engineering, environmental and biological applications



Doctoral Training Centre
Next Generation Computational Modelling (2014-2022)

- 4-year PhD programme for 75 students with taught elements
- funded by EPSRC, industry & university (£10m)

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Develop the future of simulation.

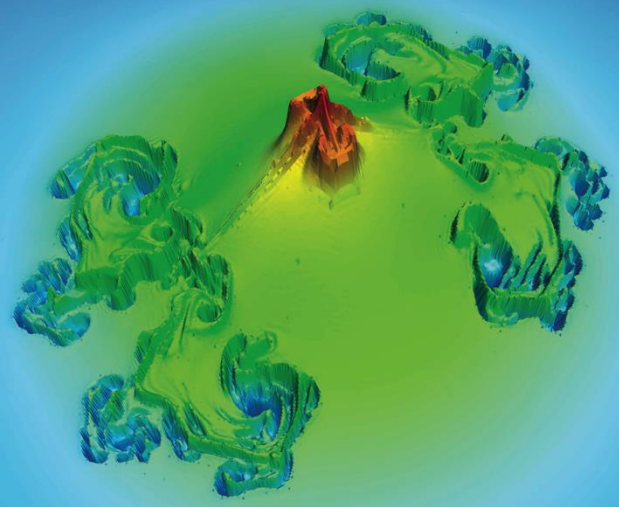
Next Generation Computational Modelling

- high performance computing
- state-of-the-art simulation methods
- writing research codes
- robust software engineering
- applications with impact

Join us at the EPSRC Centre for Doctoral Training in Next Generation Computational Modelling

Contact: ngcm@soton.ac.uk

www.ngcm.soton.ac.uk



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Case studies

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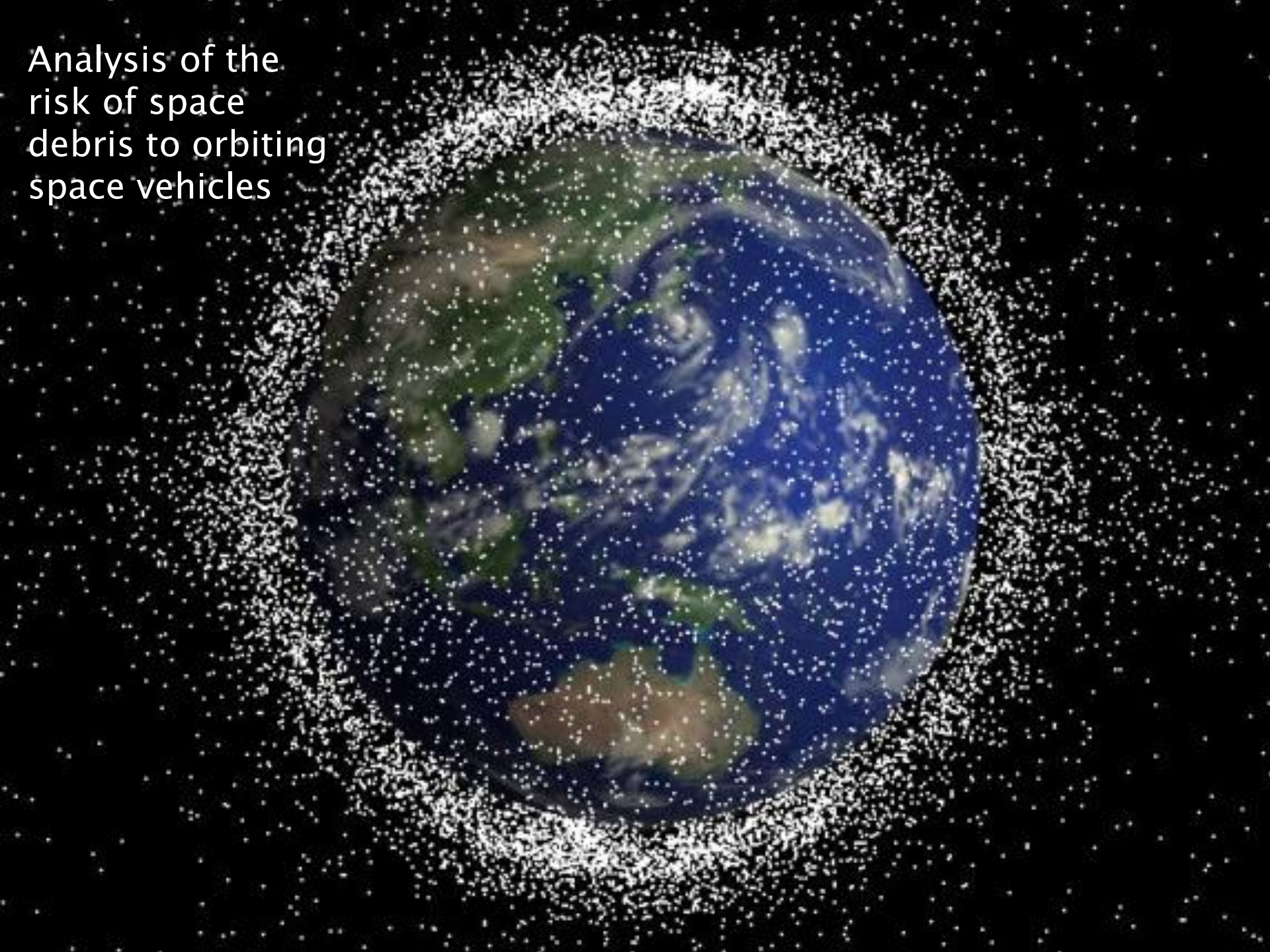
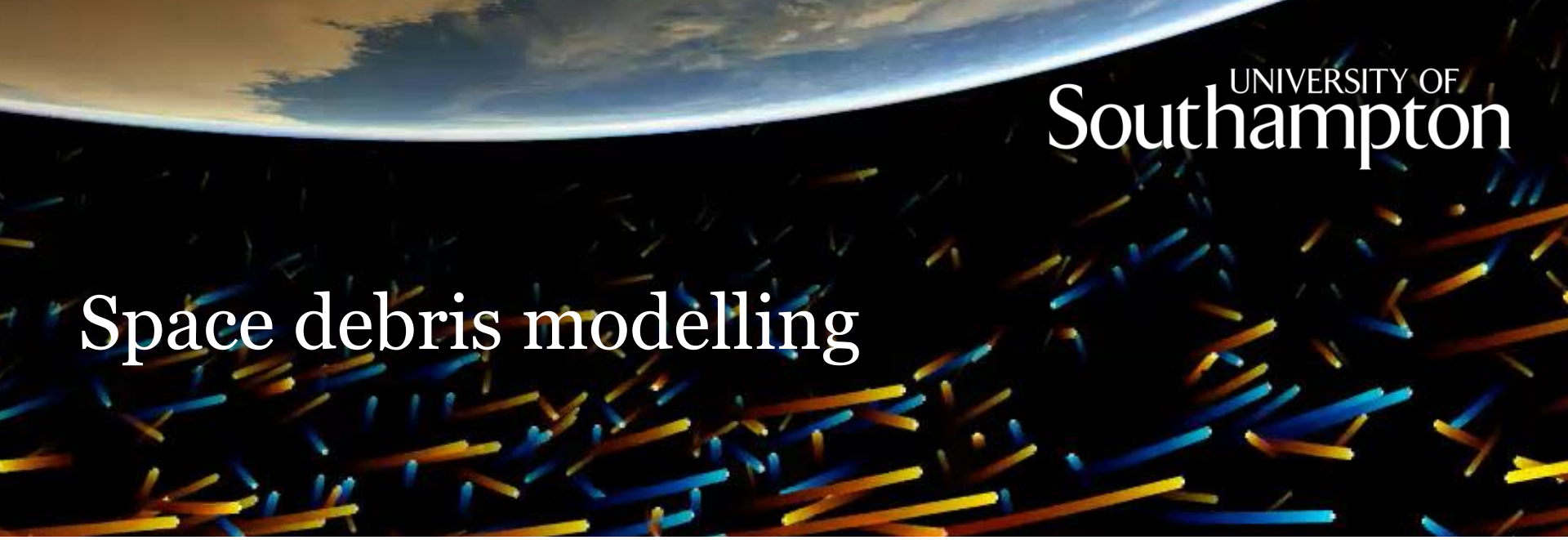
Exploring Space


Analysis of the
risk of space
debris to orbiting
space vehicles



Space debris modelling

- Space debris modelling – DAMAGE
- Space debris removal and asteroid deflection concepts
- Space Surveillance and Tracking Services
- Orbit manipulation and deflection of Near Earth Objects

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Computational Fluid Dynamics

Computational Aerodynamics

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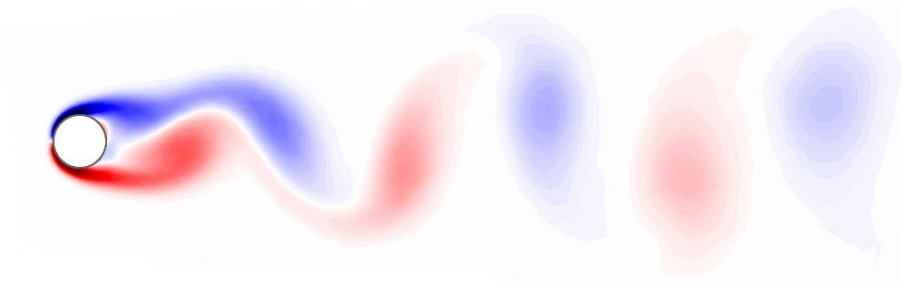
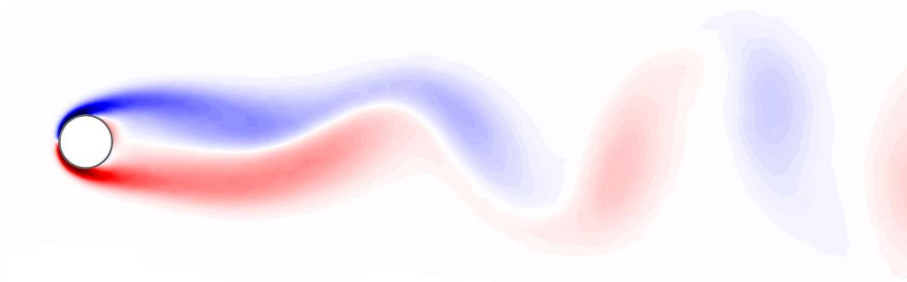
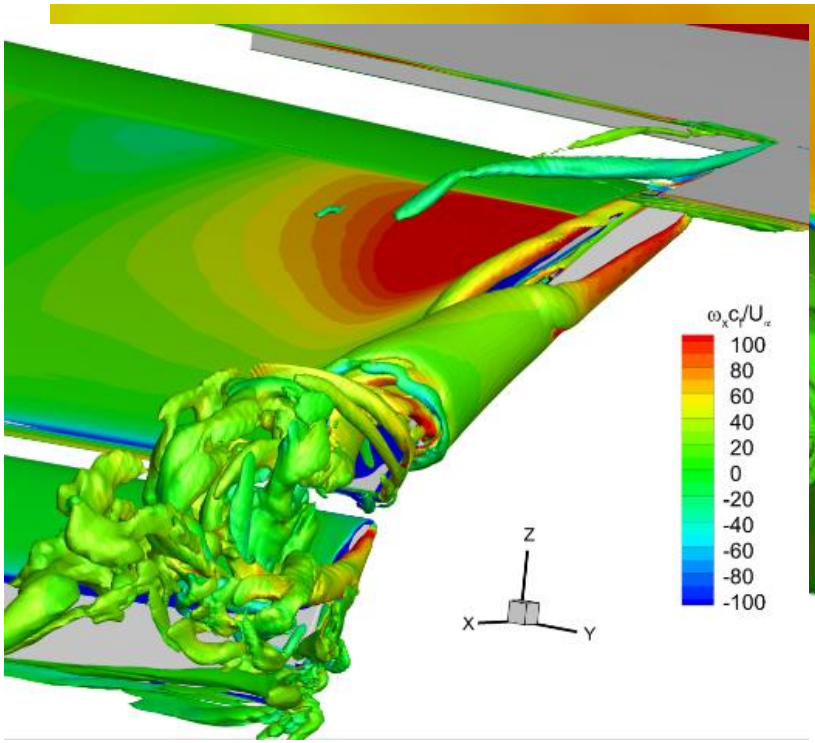
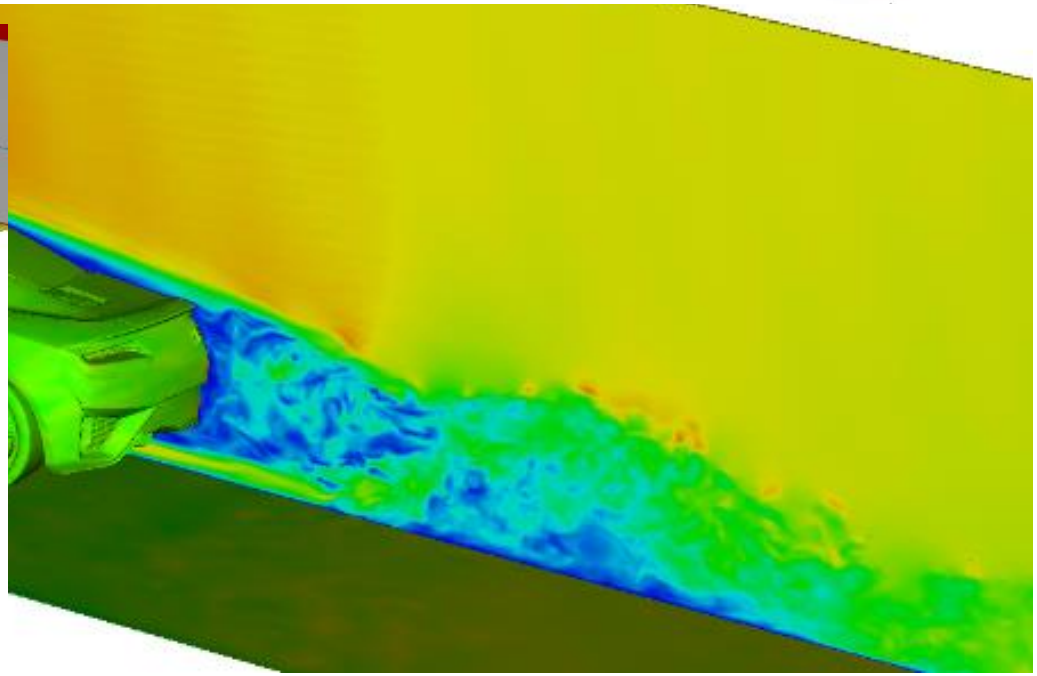
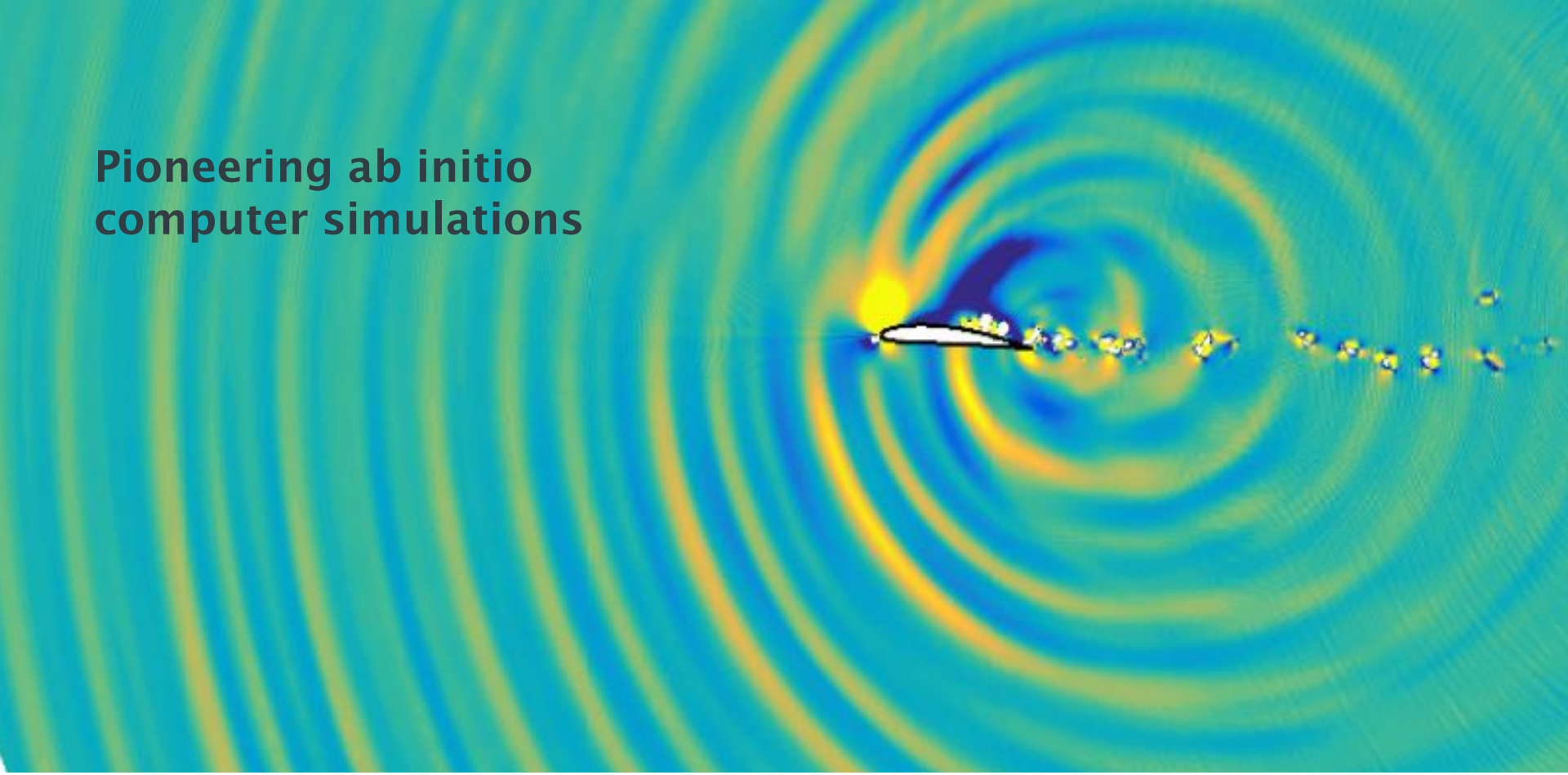


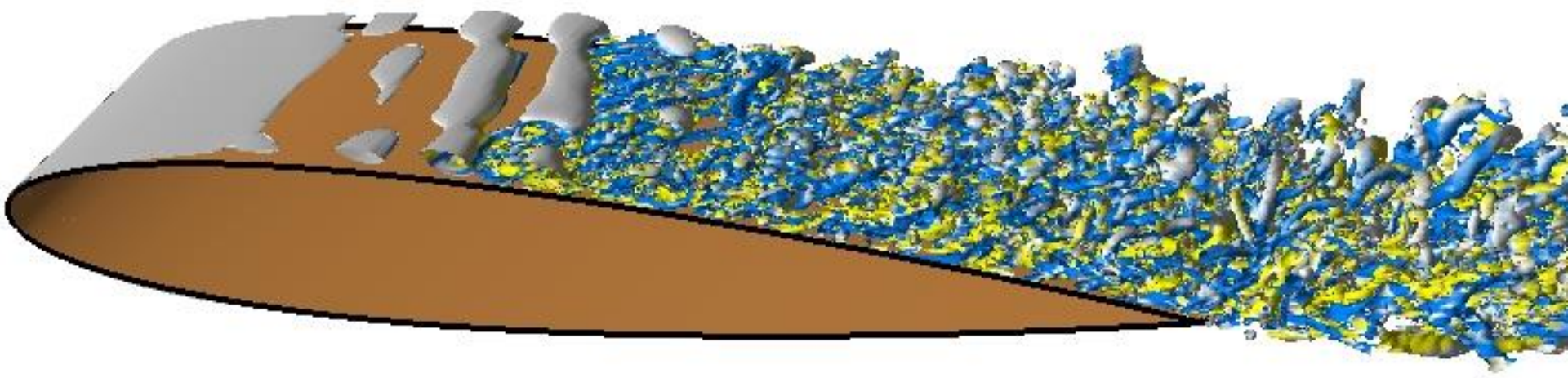






Pioneering ab initio computer simulations





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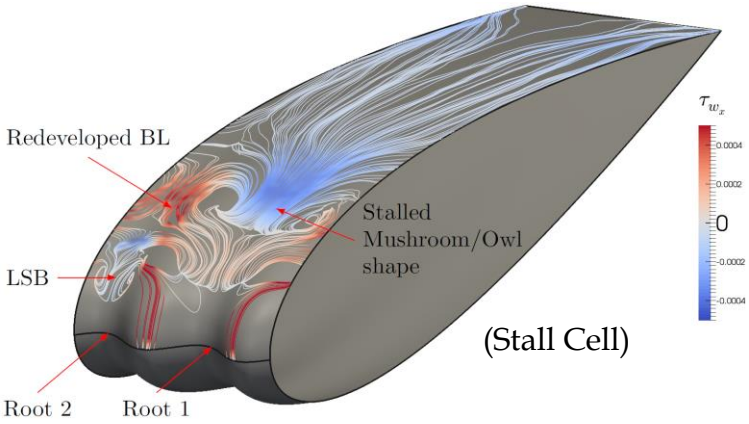
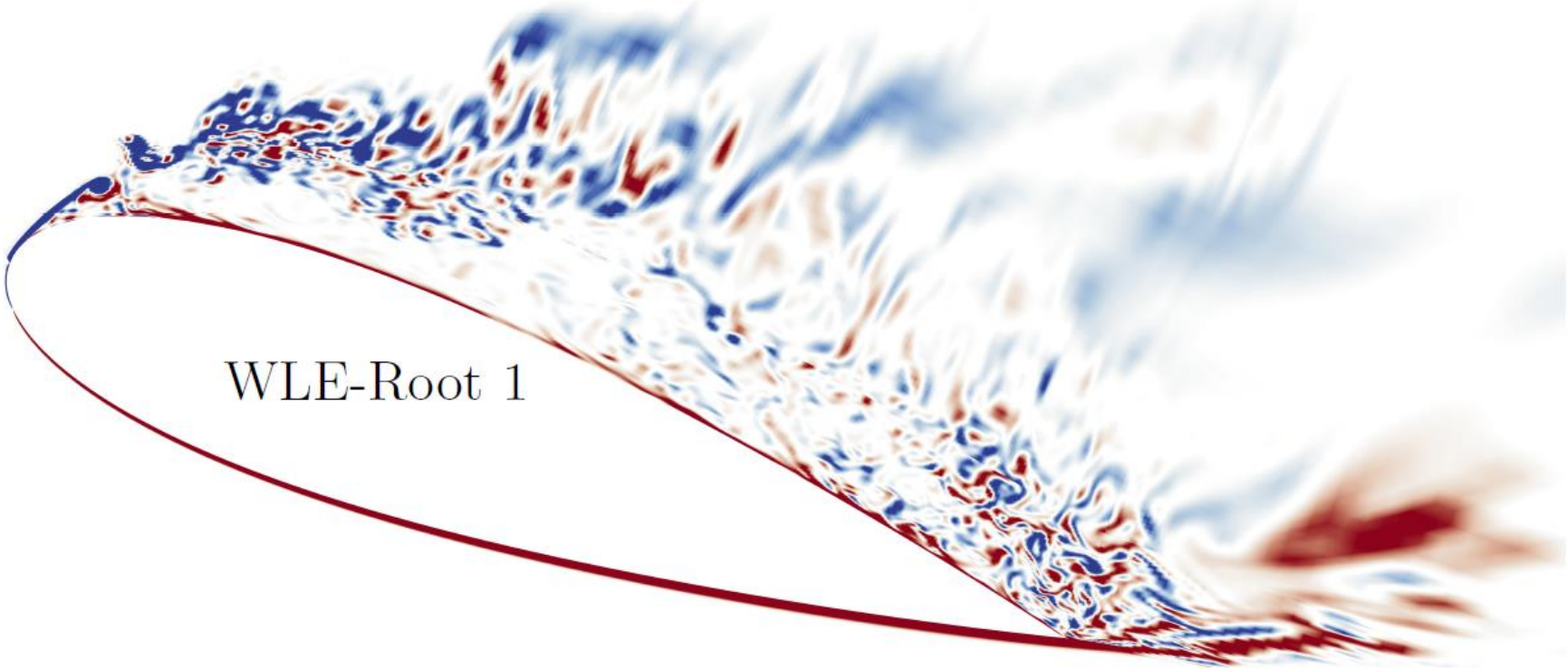
Noise and flow control

- Large Eddy Simulations
- Numerical methods
- Computational Aeroacoustics



(Stall Cell)



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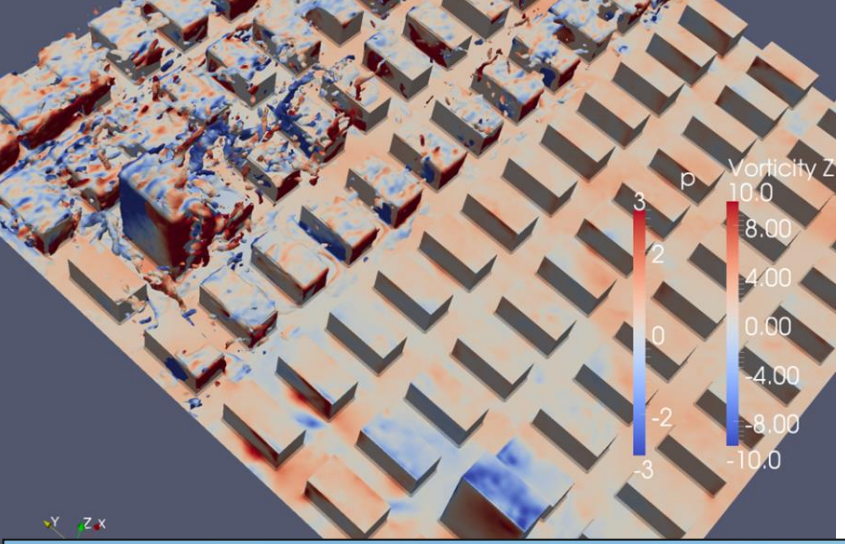
Predicting wind flows in cities

We are researching the effect of local winds on the loading on man-made structures and on the dispersion of pollutants in cities using high powered computer simulations



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- Modelling City Scale Environments
- Airborne Hazard Emergency Management

Pollution in London

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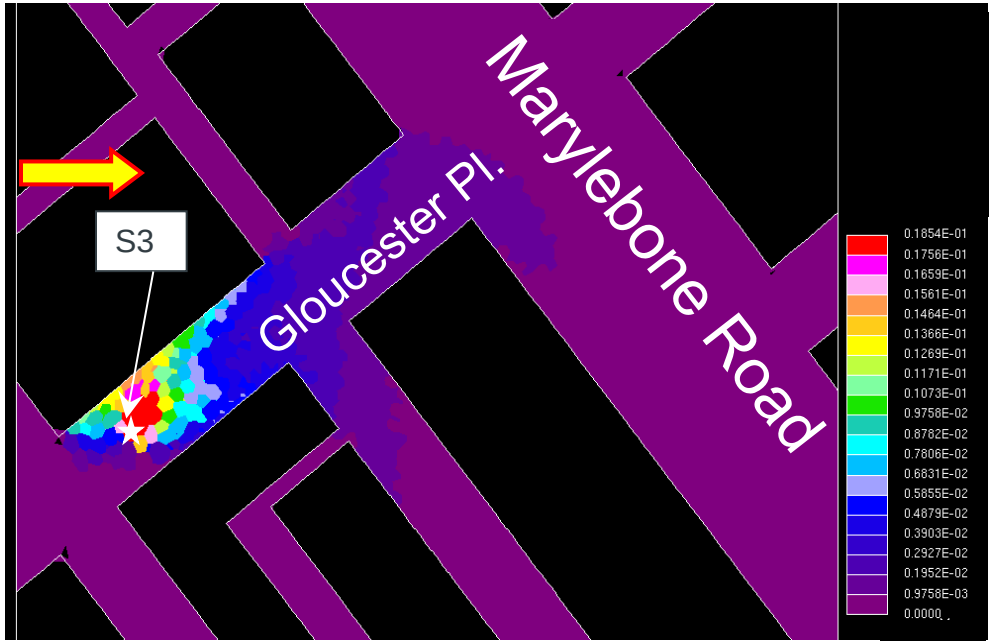
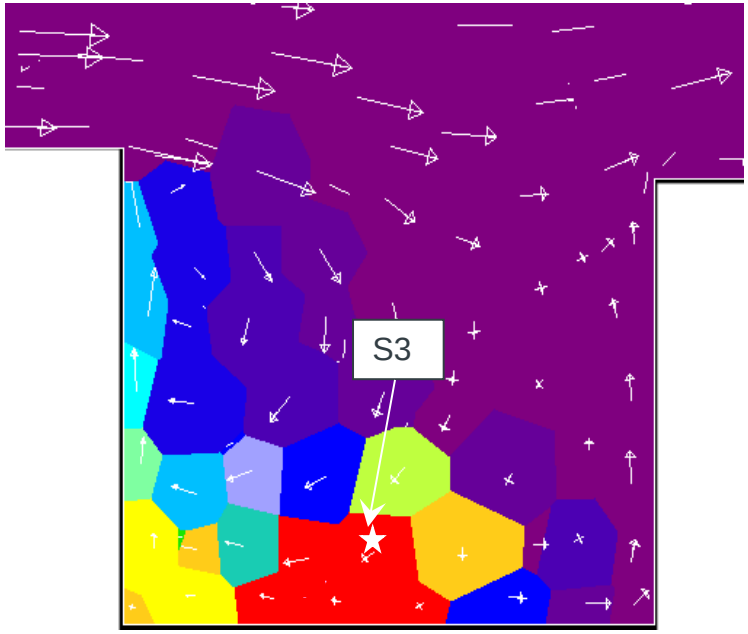


(a)

Time-mean values of pollutant level at pedestrian height from a source (S3) at the same height near a building.



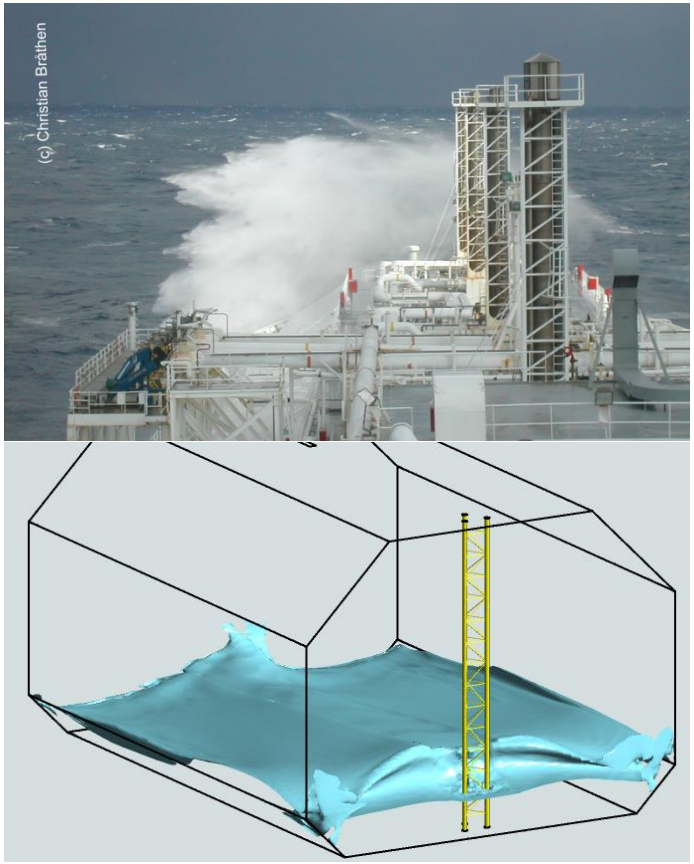
(b)

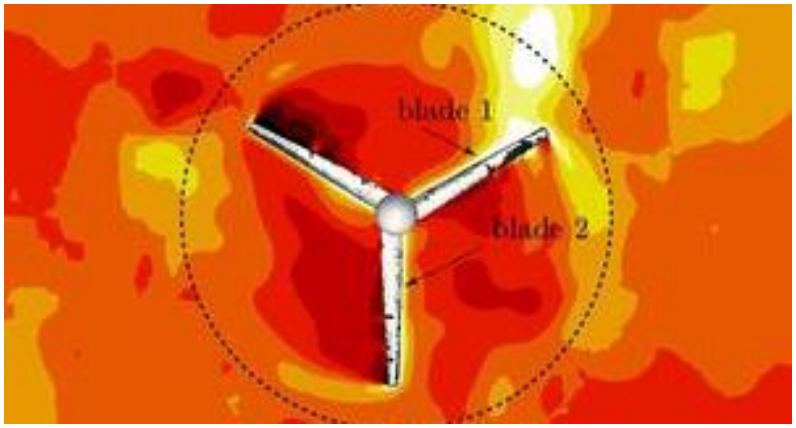
As (a), but on a vertical plane through source and perpendicular to Gloucester Place, looking towards Marylebone Road.

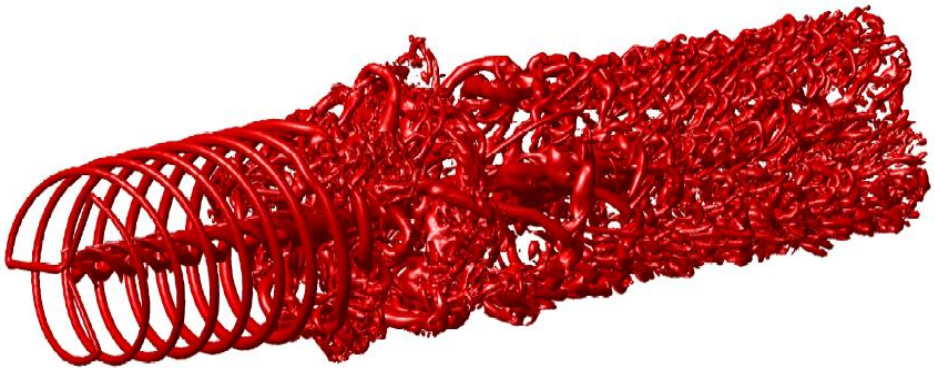
From Large Eddy Simulations, performed with support by the NERC National Centre for Atmospheric

Maritime

- Sloshing (violent fluid motion in a partially filled container under external excitation) in LNG carriers
- Performance







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Aerospace engineering

Parametric aircraft geometry modelling

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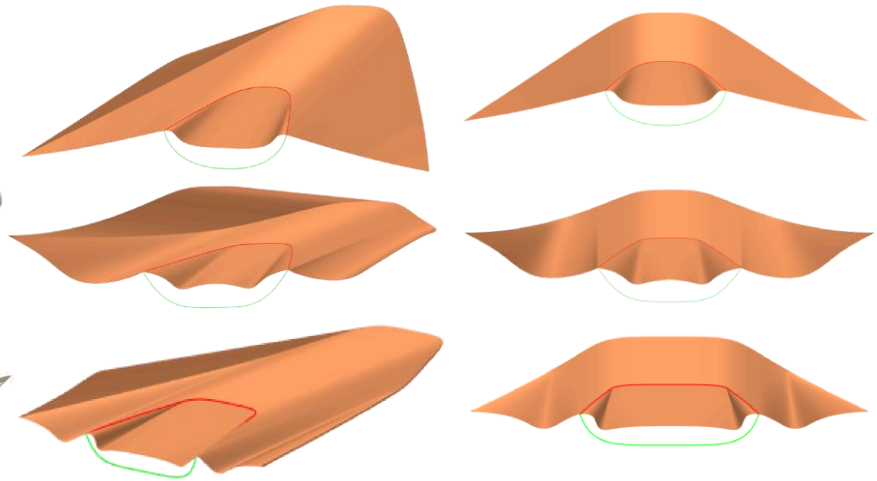

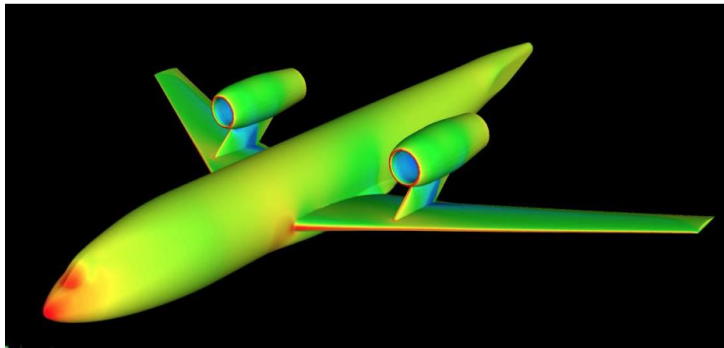

Our aeronautics and astronautics students have designed and built an ‘Octocoptor’ as part of their group design project

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Design and control of Autonomous systems

Autonomous Systems at Southampton

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- £3m capital award funding 2014
- £200k ATI funded Airbus led AIRSTART funding
- £2.5M NERC/ EPSRC funded DTC (NEXUSS; NEXt generation Unmanned System Science)

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Healthcare and building better bodies

Biomedical Engineering

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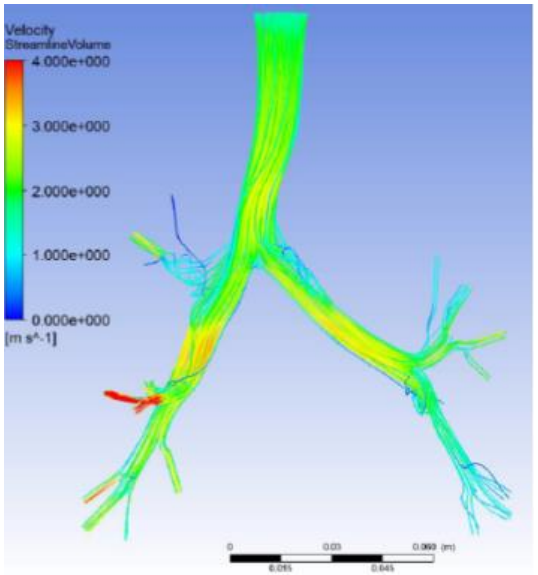
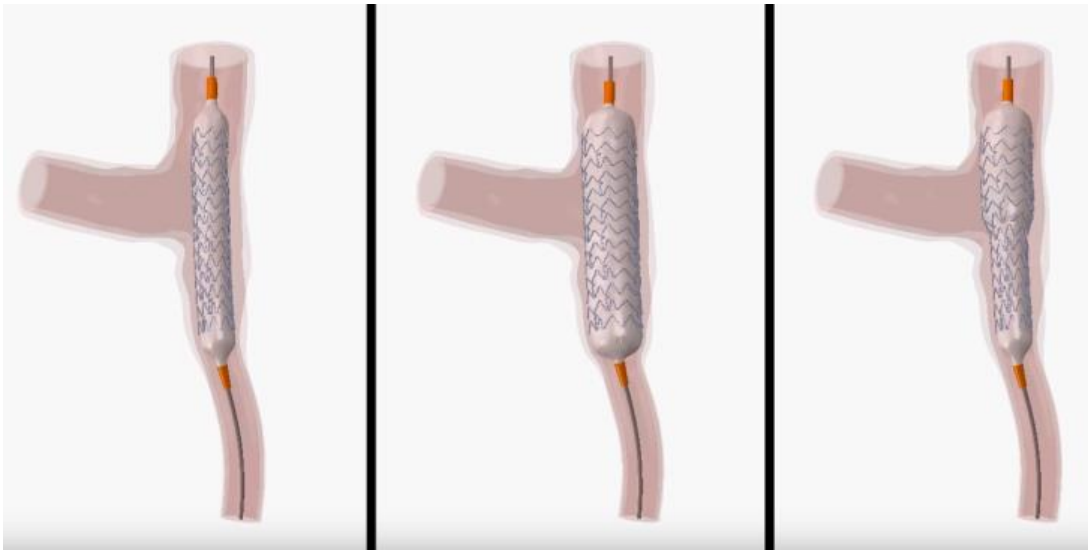
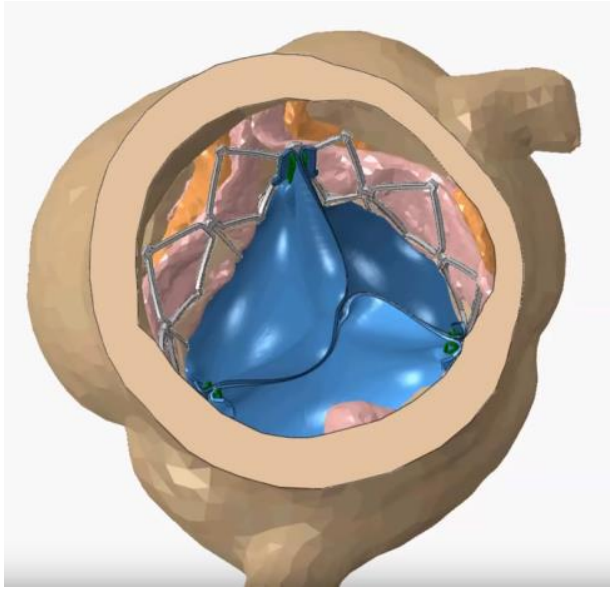
- Coronary artery stent delivery systems
- Replacement heart valve design
- Haemodynamics in the human heart
- Multi-scale modelling of the human lung







Magnetic nano particles for diagnostics and healthcare

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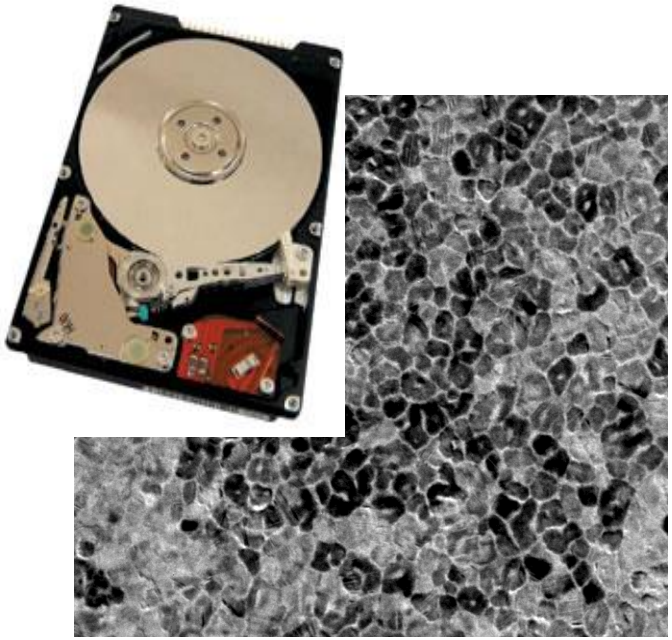
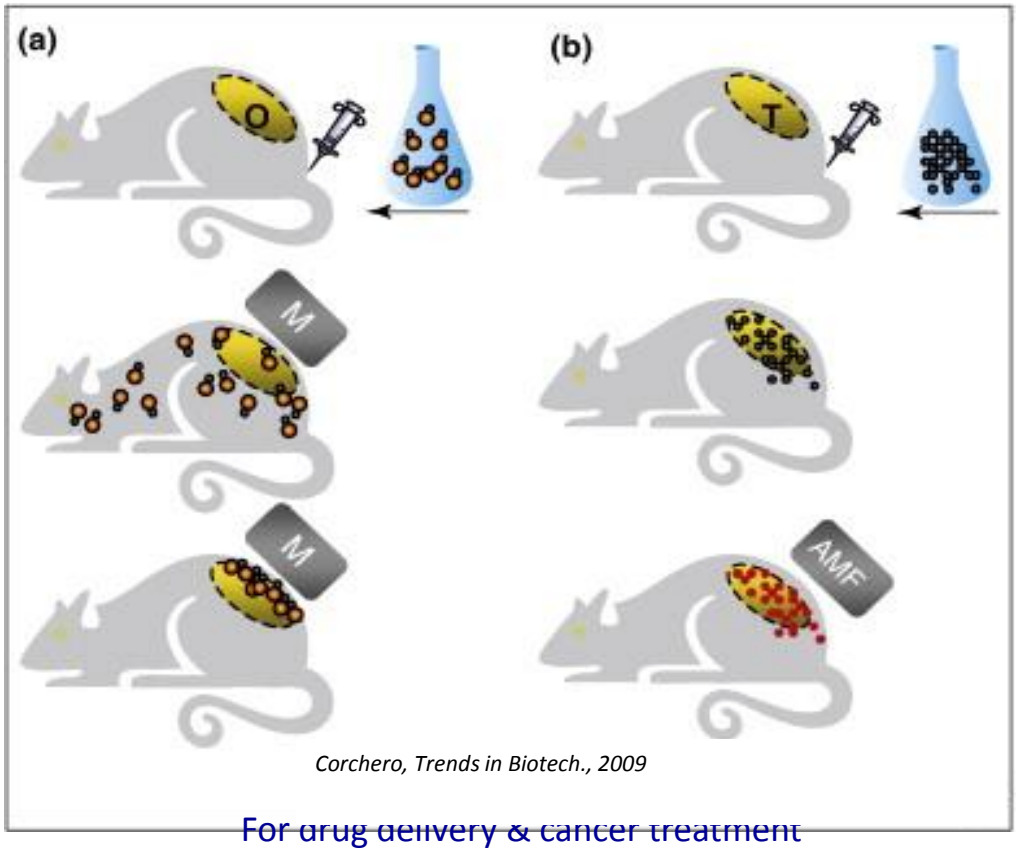
- Applications in
  - sensing & imaging methods
  - Targetted drug delivery in human body
  - Thermal cancer treatment





Corchero, Trends in Biotech., 2009

For drug delivery & cancer treatment

Ultrasonics in microfluidics – point of care diagnostics

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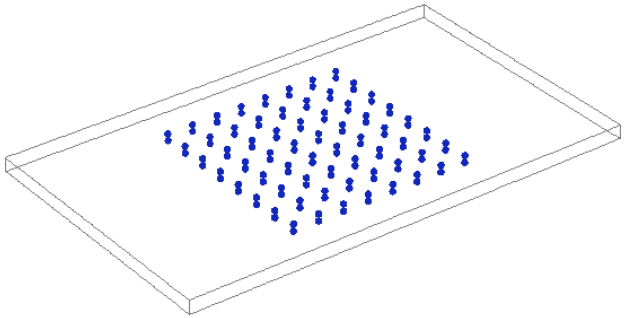
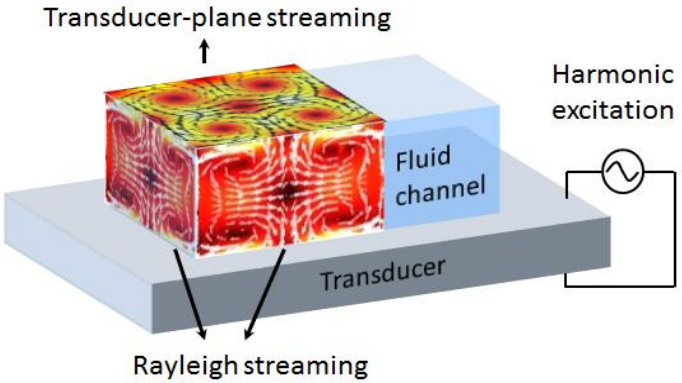
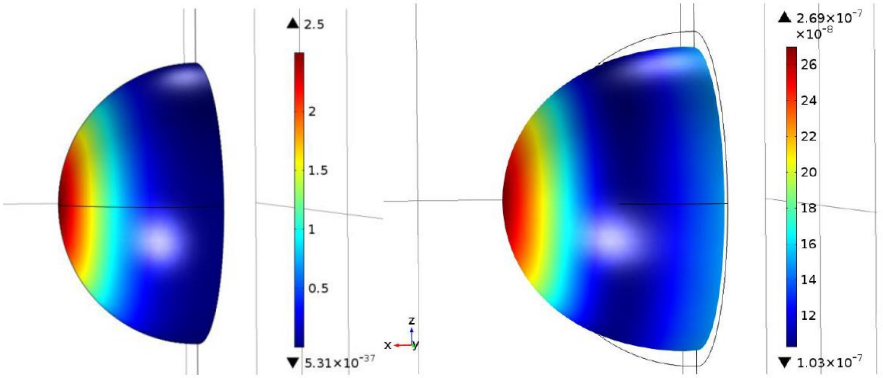
Ultrasound can levitate, manipulate, and stimulate cells and mix fluids.





Acoustic streaming fields

Multiscale, multi-physics modelling is required to predict behaviour



Cell mechanical characterisation

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Computational Chemistry

Multiscale chemistry modelling

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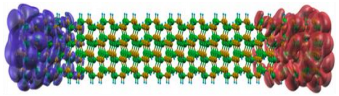


Complexity

Quantum
Atomistic

Hybrid coarse-grain/atomistic continuum

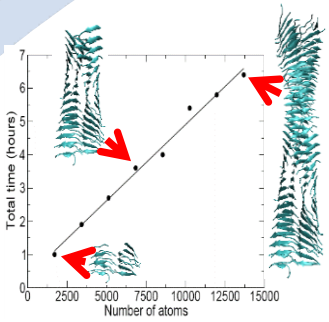
Coarse-grain

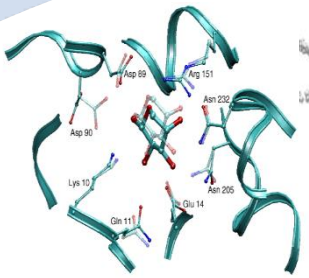
Materials Crystal Structure

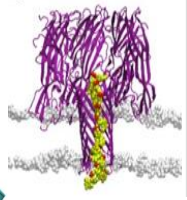
Data Driven Informatics

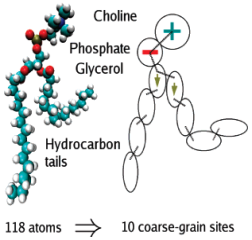
Chemical Space

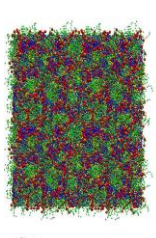
Quantum Mechanics

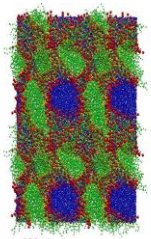


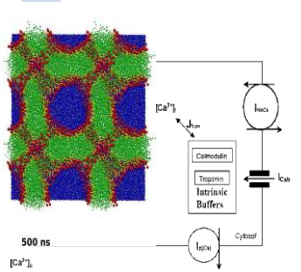


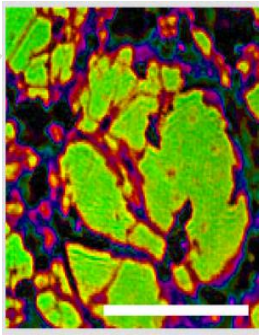












Computationally Intensive Imaging (x-ray imaging, NMR and EPR for structure and dynamics)

SIZE

Ab-initio nanoparticle simulation

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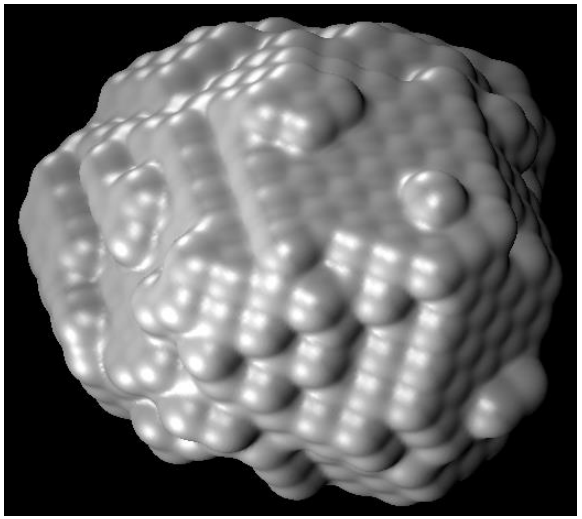
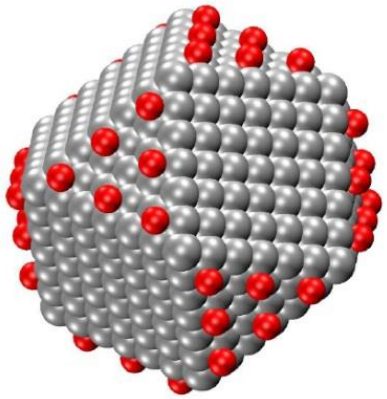
Small molecule adsorption and catalysis on Pt nanoparticles

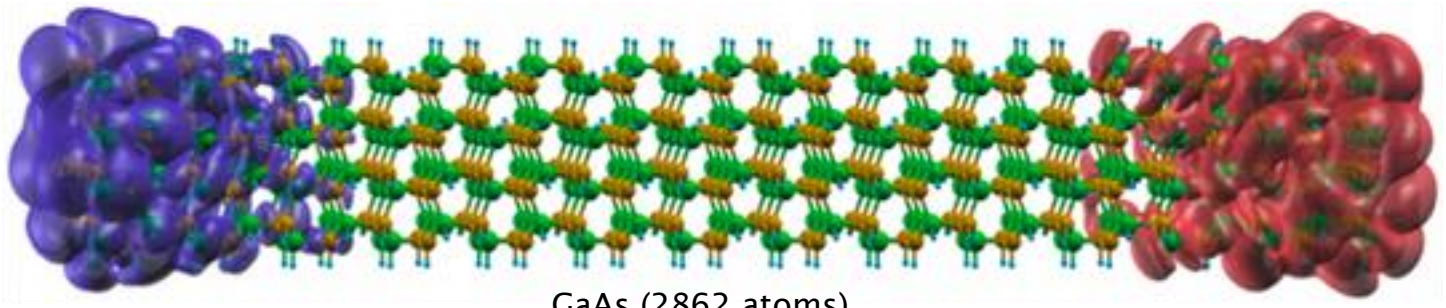


Pt_{943}



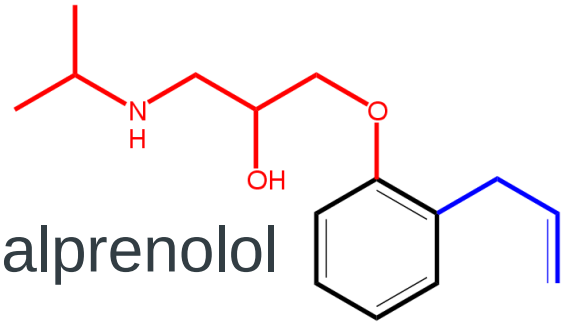
Pt_{561} with Oxygen (red) adsorbed on the (111) facets

Electronic properties of semiconductor nanorods

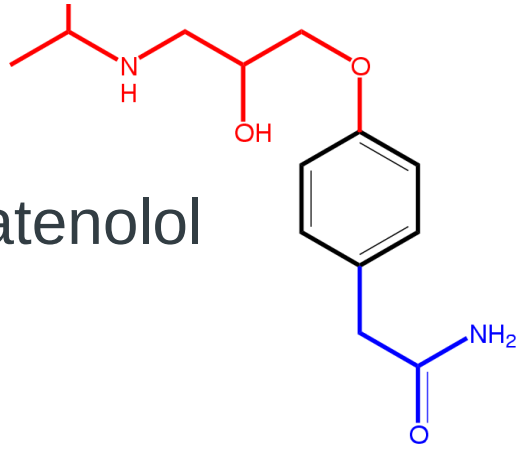


GaAs (2862 atoms)

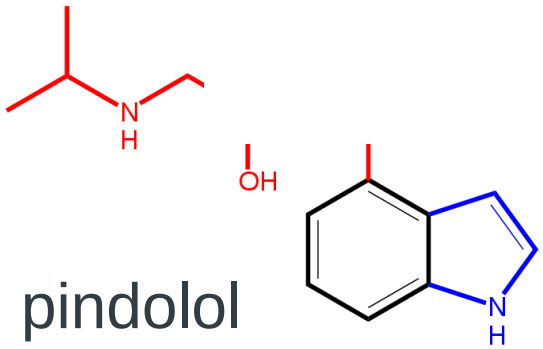
Multiscale simulation of drugs: β-blockers



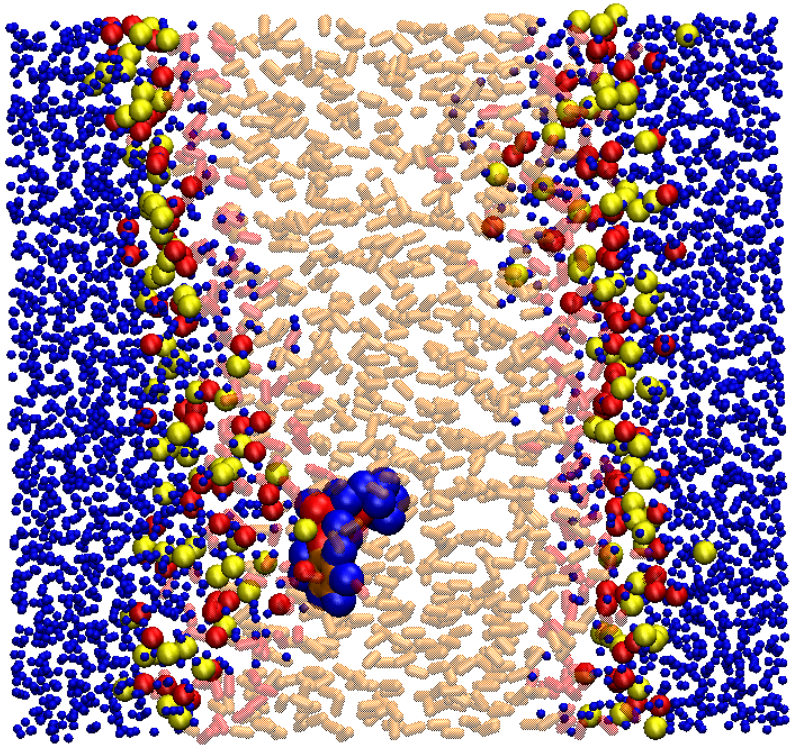
alprenolol

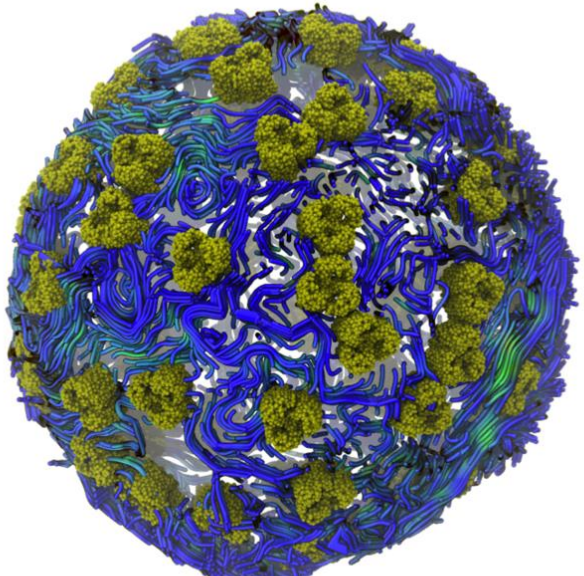


atenolol



pindolol





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Design optimisation

Design Optimisation

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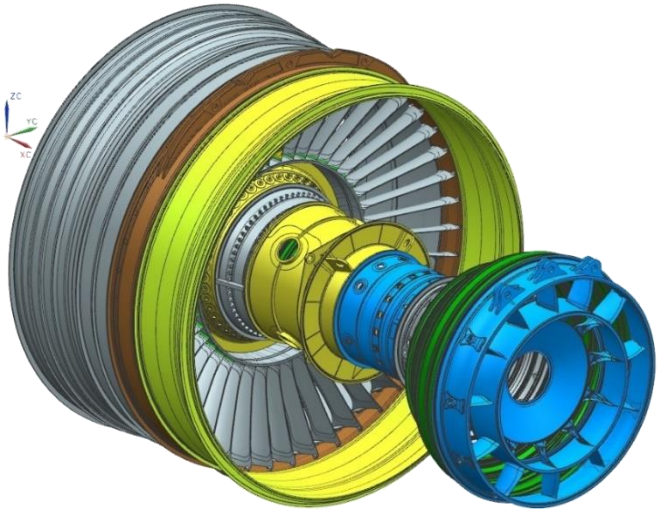
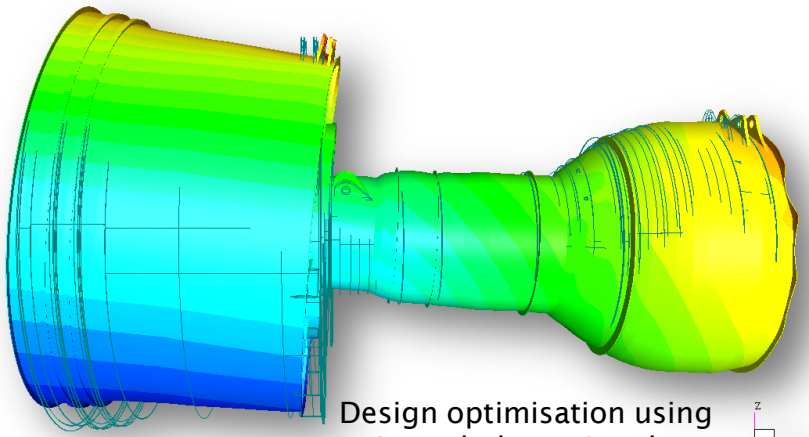
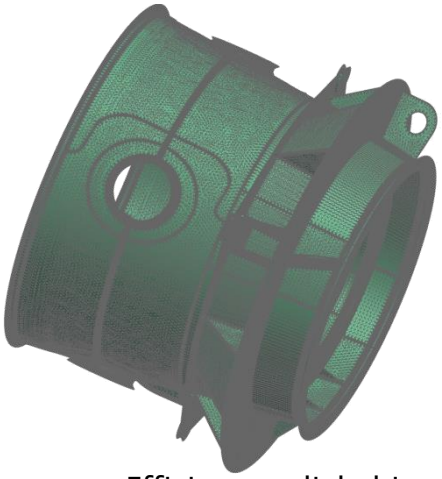
- Gas turbine design optimisation
- Multi-fidelity & non-stationary surrogate modelling
- CAD & simulation automation
- Life time optimisation of products



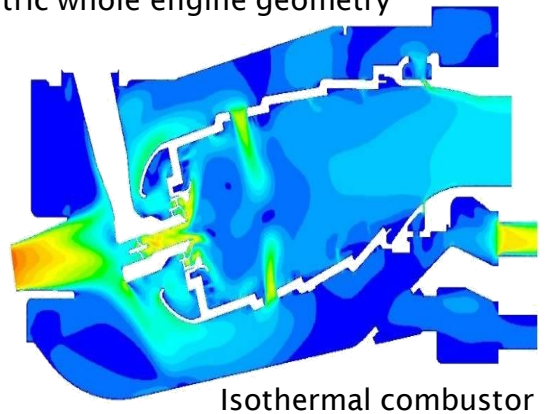
Parametric whole engine geometry



Design optimisation using transient whole engine thermo-mechanical analyses



Efficient medial object transformation



Isothermal combustor design optimisation

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Materials and multi-physics

Advanced materials research

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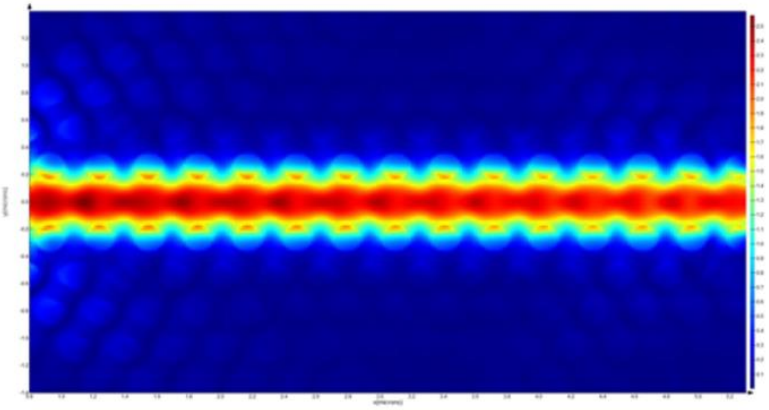
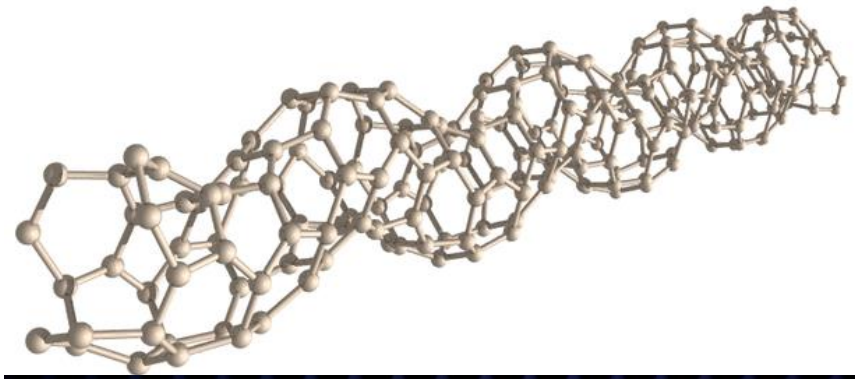
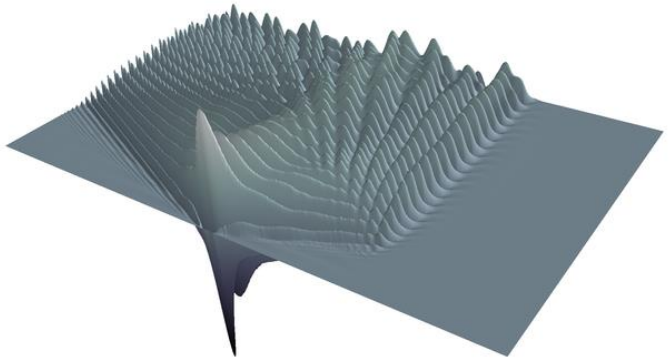
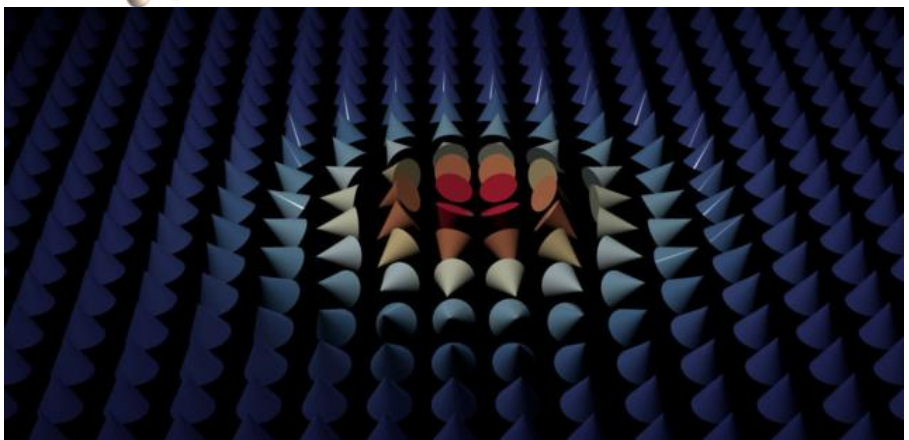
- Photonics, nanomagnetics, functional materials
- Quantum technology and nano technology devices
- Lightweight and super strength materials









Multiphysics simulations

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- Needed in many places
- Example: combustion & fire fighting

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Computational Methodology & tools for the future

Better software

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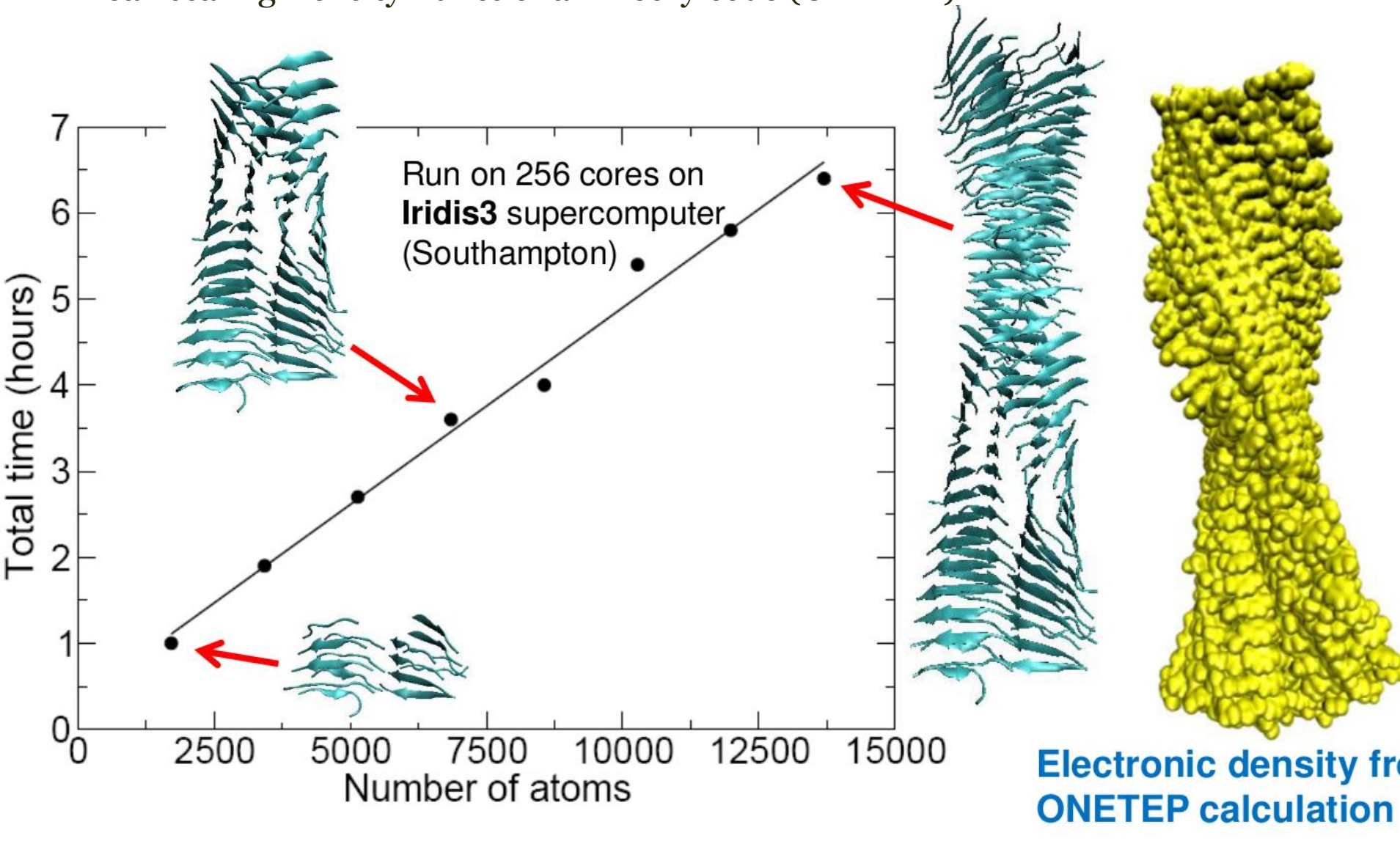
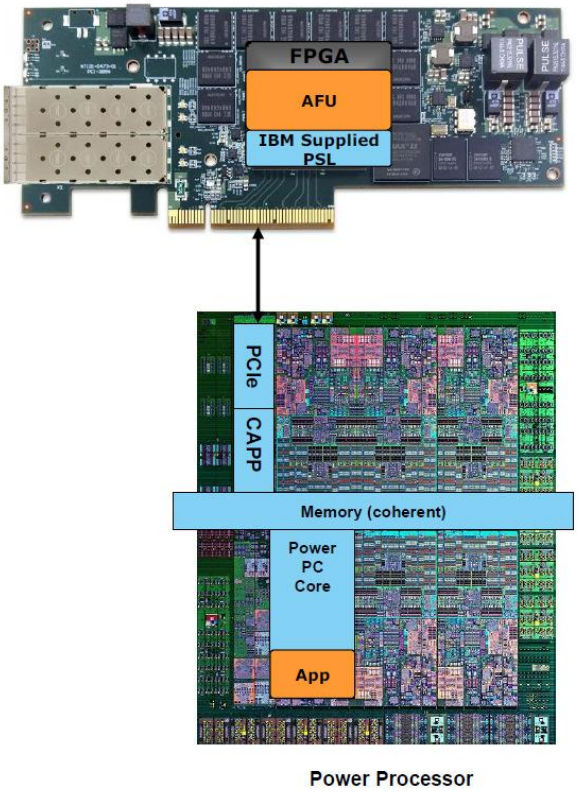
Linear-scaling Density Functional Theory code (ONETEP)



Hardware Acceleration

- CPU clock rate cannot increase further
- Performance increase through parallelisation
- Accelerators co-processors (“many-core”)
  - GPU
  - Intel Xeon Phi
  - Field Programmable Gate Array (FPGA)
- FPGAs
  - reconfigurable co-processors
  - High long term potential



IBM

Accelerating software creation

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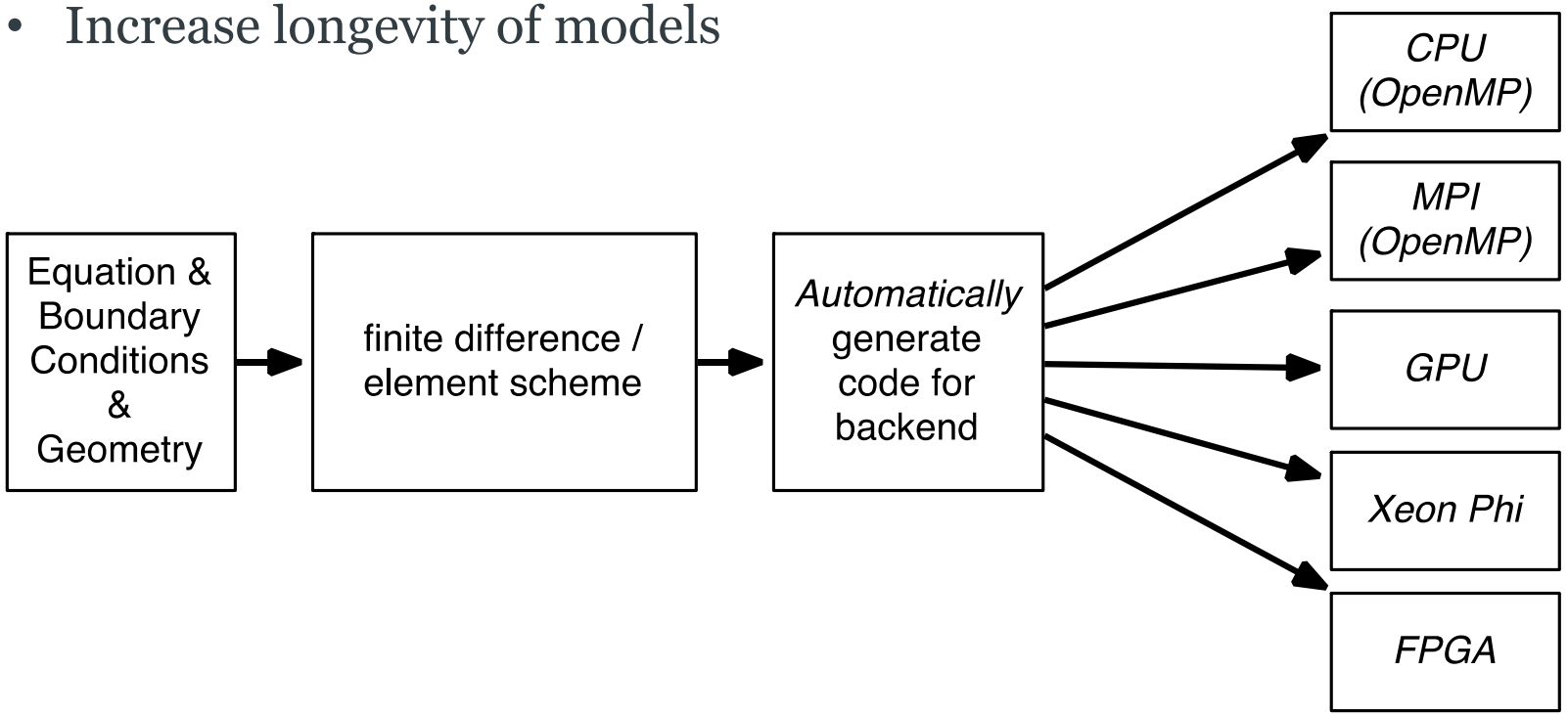
- Automatic code generation for PDE based multi-physics simulation
  - Reduce coding effort
  - Improve correctness
  - Increase execution performance
  - Increase longevity of models



Work flow tools

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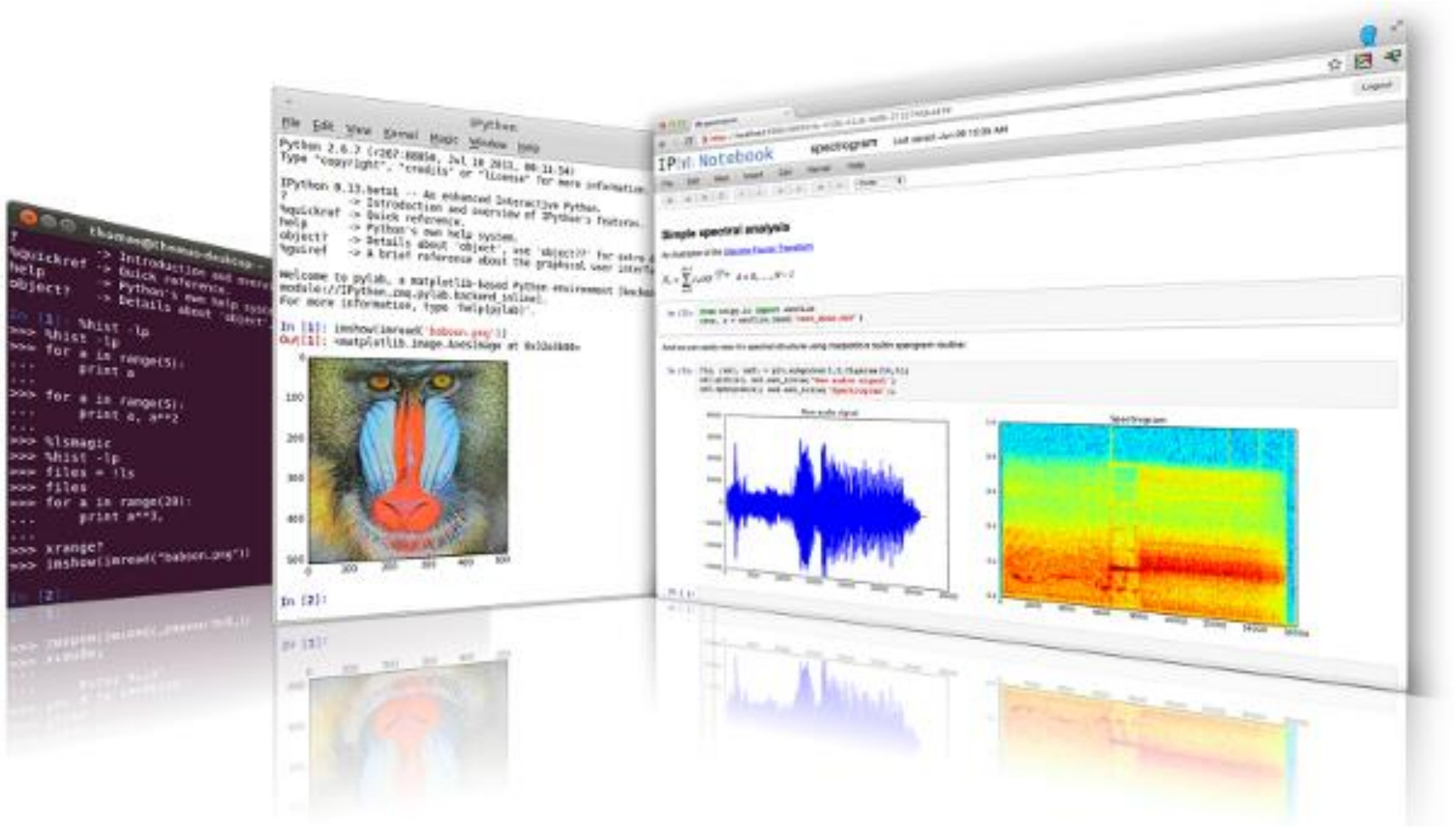
- Increase productivity by appropriate simulation and data analysis workflow tools



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Thank you

Computational Modelling Group
http://cmg.soton.ac.uk

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