Modelling and Simulation

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Professor of Computational Modelling
Computational Modelling

- 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
Computing @ University of Southampton

- Pegasus (1950’s)
- ICL (1960’s & 70’s)
- IBM 3090 (1980’s)
- IBM SP2 (1990’s)
- Iridis1-4 (2001-2013)
Mission

• 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

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

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), SimpWare (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)
Computational Resources

- 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

- 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 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

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

• 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)

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
Case studies
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
Computational Fluid Dynamics
Computational Aerodynamics
Pioneering ab initio computer simulations
Noise and flow control

- Large Eddy Simulations
- Numerical methods
- Computational Aeroacoustics
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.
- Modelling City Scale Environments
- Airborne Hazard Emergency Management
Pollution in London

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

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
Aerospace engineering
Parametric aircraft geometry modelling
Our aeronautics and astronautics students have designed and built an ‘Octocoptor’ as part of their group design project.
Design and control of Autonomous systems
Autonomous Systems at Southampton

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

- 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

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

*Corchero, Trends in Biotech., 2009*
Ultrasonics in microfluidics – point of care diagnostics

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

Multiscale, multi-physics modelling is required to predict behaviour

Cell mechanical characterisation

Acoustic streaming fields
Computational Chemistry
Multiscale chemistry modelling

Complexity

Quantum Mechanics

Atomistic

Hybrid coarse-grain/atomistic continuum

Coarse-grain

Materials Crystal Structure Prediction

Data Driven Informatics

Chemical Space

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

SIZE
Ab-initio nanoparticle simulation

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
Design optimisation
Design Optimisation

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

- Design optimisation using transient whole engine thermo-mechanical analyses
- Efficient medial object transformation
- Isothermal combustor design optimisation
- Parametric whole engine geometry
Materials and multi-physics
Advanced materials research

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

- Needed in many places
- Example: combustion & fire fighting
Computational Methodology & tools for the future
Better software

Linear-scaling Density Functional Theory code (ONETEP)

Run on 256 cores on Iridis3 supercomputer (Southampton)

Electronic density from ONETEP calculation
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
Accelerating software creation

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

• Increase productivity by appropriate simulation and data analysis workflow tools
Thank you

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