



Centre for Doctoral Training in

Next Generation Computational Modelling

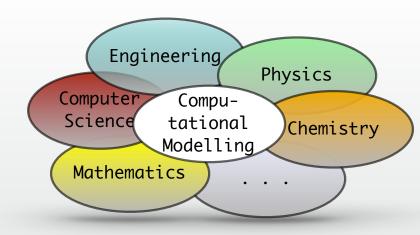
Hans Fangohr, Ian Hawke, Peter Horak EPSRC Centre for Doctoral Training





CDT in Next Generation Computational Modelling (NGCM) – why?

- Computer simulation underpins research and development in science and engineering in academia and industry, for example:
 - Understanding measurements
 - Predicting measurements and performance
 - Improving materials, designs, devices, treatment, policies.
 - Cutting R&D costs.

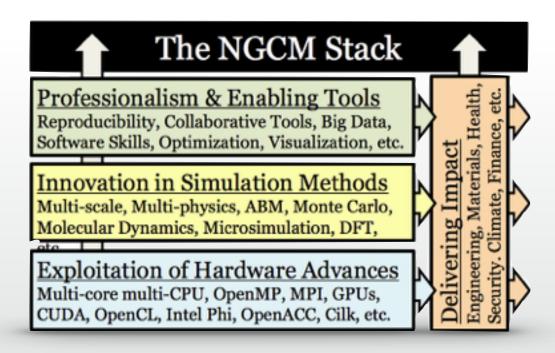






CDT in Next Generation Computational Modelling (NGCM) – what?

- Training and research addressing
 - professionalism
 - simulation methods
 - exploitation of latest hardware







Next Generation Computational Modelling CDT

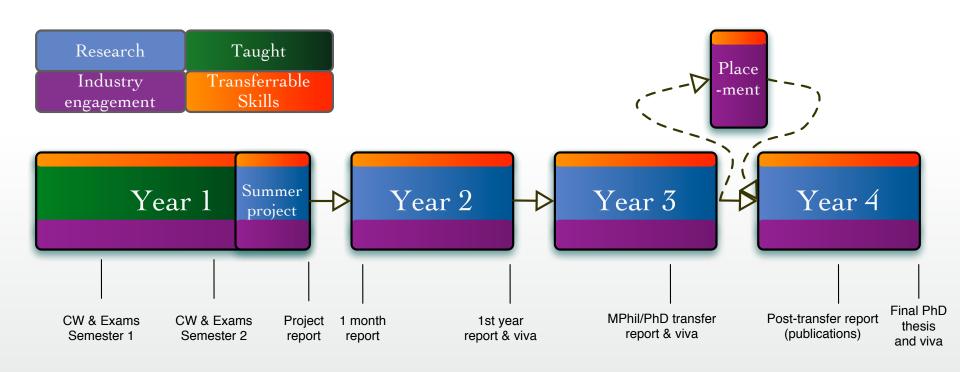
- Funded by the
 Engineering and Physical
 Science Research Council
 (EPSRC), with
 contributions from
 industry and University of
 Southampton,
 total ~ £10 million
- 15 studentships for UK/ EU students to start every year (from 2014 to 2018)







4-year programme, overview





First year training programme

- 6 compulsory modules (90 credits)
- 2 optional modules (30 credits)
- Summer project (60 credits)
- Required pass mark for funding at end of year 1: 60%, 65% in summer project

Python Programming Primer (one week)

IV

Modelling and Simulation

Ab-initio (DFT), Molecular Dynamics, Monte Carlo, Finite Elements, Agent-based, discrete event, stochastic differential equations

Computational Methods I

Compiled code, C
Programming, symbolic
computation, linking
Python and C,
autogeneration of code

Numerical Methods

Numerical analysis, linear algebra, quadrature, ordinary and partial differential equations.

Semester 2, 60 credits

Semester 1, 60 credits

Statistics for Computational Modelling

Data and statistical analysis, hypothesis testing, inference, design of experiments.

Computational Methods II

Parellel programming (OpenMP, MPI), visualisation, testing, reproducibility, software engineering

Professional and Research Skills*

Transferrable skills, communication, team work. Computational modelling contextualised, and summer project preparation.

Summer, 60 credits

NGCM Summer Academy (one week)

Summer project (three months)

Mini research project with industry focus

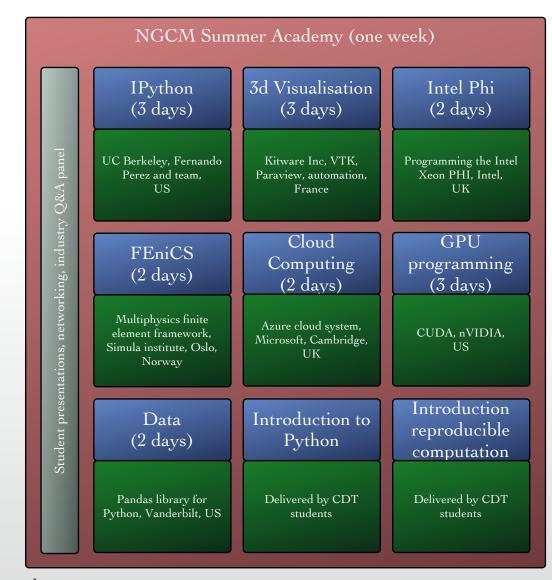
Web: http://ngcm.soton.ac.uk - Email: ngcm@soton.ac.uk





Summer Academy

- Annual meeting from summer 2015 onwards
- Open for participation from outside Southampton
- Parallel training sessions (examples on the right)
- High profile international trainers
- Centre of gravity for computational modelling in the UK
- http://ngcm.soton.ac.uk/ summer-academy/







Facilities:

Southampton Supercomputer Iridis

- £3.2 million investment in 2013
- hardware refresh cycle of 3 years
- part of 10-year strategy plan for High Performance Computing (HPC), i.e. long-term commitment of university







Facilities:

Access to National supercomputer ARCHER

- ARCHER (Advanced Research Computing High End Resource)
- 72,192 cores Cray XC30
- 1,367.5 TFlop/s
- 12-core 2.7GHz Intel E5-2697 v2 (Ivy Bridge)
- Network is the new Cray Aries interconnect

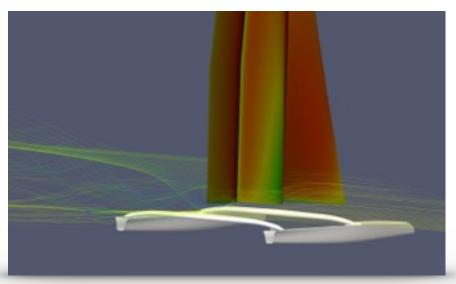


• Rank 19 in top 500
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Other Facilities:

- 372 NVIDIA GPUs at Emerald, 114 TF compute power, Jointly used with Oxford, Bristol, and UCL
- Dedicated for CDT:
 - New 134k GPU machine at Southampton
 - New ARM and Power8 architectures and x86 cluster (worth ~250k)







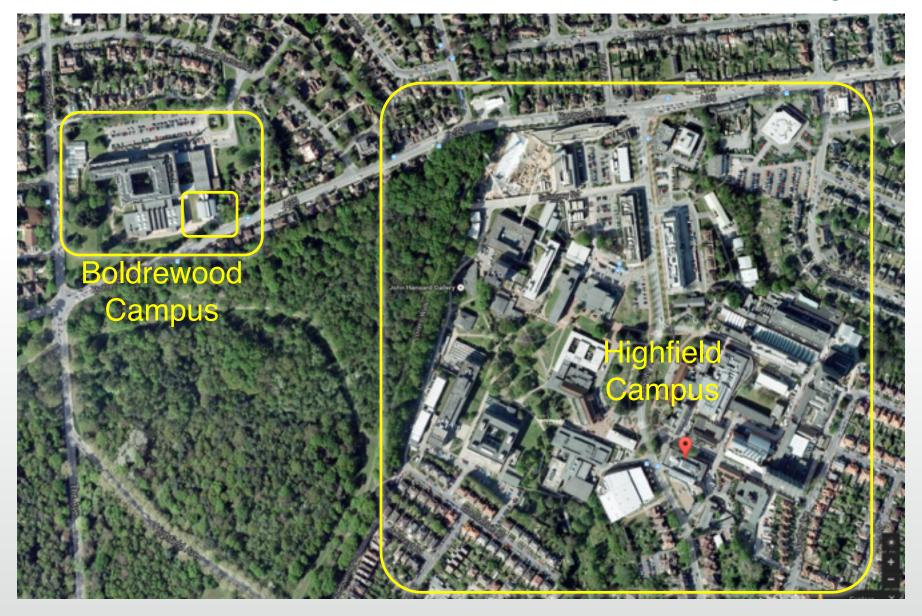


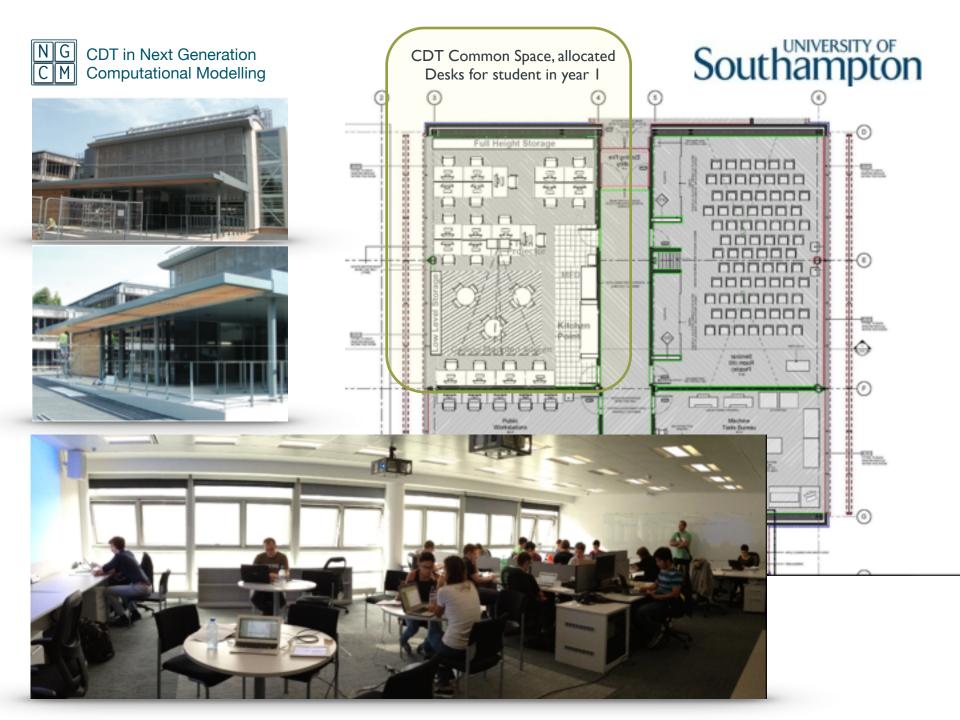
CDT located on newly developed Boldrewood campus complex

- £116m investment
- Campus Completion in Summer 2014
- Hosting all computational engineering
- Dedicated space for NGCM CDT students







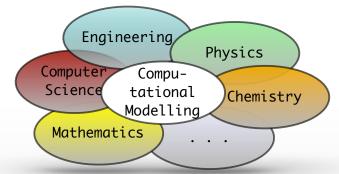






Supervisors from Computational Modelling Group

- > 170 academic staff
- > 600 post-docs and PhD
- use computer simulation to advance <u>research and engineering</u>
- joint seminars, training, research
- interdisciplinary networking
- Details: http://cmg.soton.ac.uk



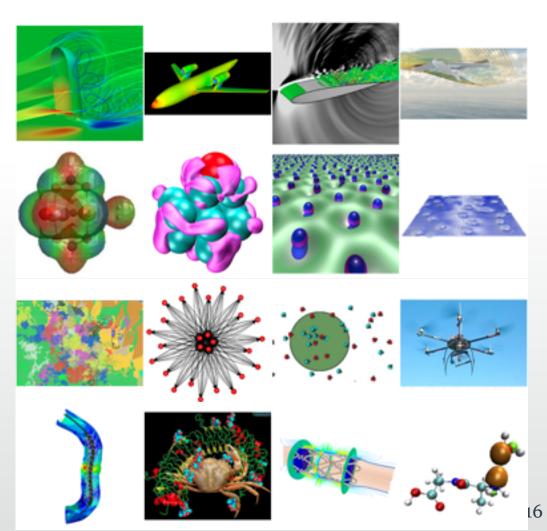






NGCM Research focus areas

- Computational Engineering
- Advanced Materials
- Autonomous Systems
- Biomedicine and Healthcare





NGCM projects



- Computer simulations of magnetic skyrmions
- Modelling the flow of glass during the draw of microstructure optical fibres
- Modelling jet dynamics at the Large Hadron Collider
- Design and simulation of reconfigurable optical fibres
- Robust design of UAV anti-vibration systems
- Simulations of chemistry at the nanoscale using first principles quantum mechanics
- Computational modelling of the dynamic interaction between the human body and a car seat
- Towards decoding the fundamental theory of nature at the Large Hadron Collider
- Teams of autonomous agents
- Challenging topological prejudice automated airframe layout design
- High-fidelity simulations of the interaction of freestream turbulence with turbulent boundary layers
- Simulation of biological systems at long length and distance scales
- Computational modelling of underwater noise generation by turbulent fluid-structure interactions
- Clean combustion of hydrogen-rich alternative fuels at high pressure
- Agent-based modelling of high frequency traders
- Multi-scale modelling of Composite Riser Systems
- Towards airborne hazard emergency management system for local environments
- Dispersion of small inertial particles in characteristic atmospheric boundary layer Web: http://ngcm.soton.ac.uk Email: ngcm@soton.ac.uk





Applications from students invited now to start September 2015

- Expect normally 1st class degree
- Background in Maths, Physics, Engineering, Chemistry, Computer Science
- Interest in simulation and programming
- Some background in Programming
- Apply at http://ngcm.soton.ac.uk/apply.html





Application process

- Identify suitable project(s) on http://ngcm.soton.ac.uk (or email ngcm@soton.ac.uk for advice)
- Email application materials to ngcm@soton.ac.uk
- If shortlisted, attend interview at Southampton



Contact

- Email: ngcm@soton.ac.uk
- Website: <u>ngcm.soton.ac.uk</u>
- Blog: ngcm.soton.ac.uk/blog
- Twitter: @ngcm_soton
- Phone: 023 8059 1272

Southampton

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

