CDT in Next Generation Computational Modelling

EPSRC
Engineering and Physical Sciences Research Council

UNIVERSITY OF Southampton

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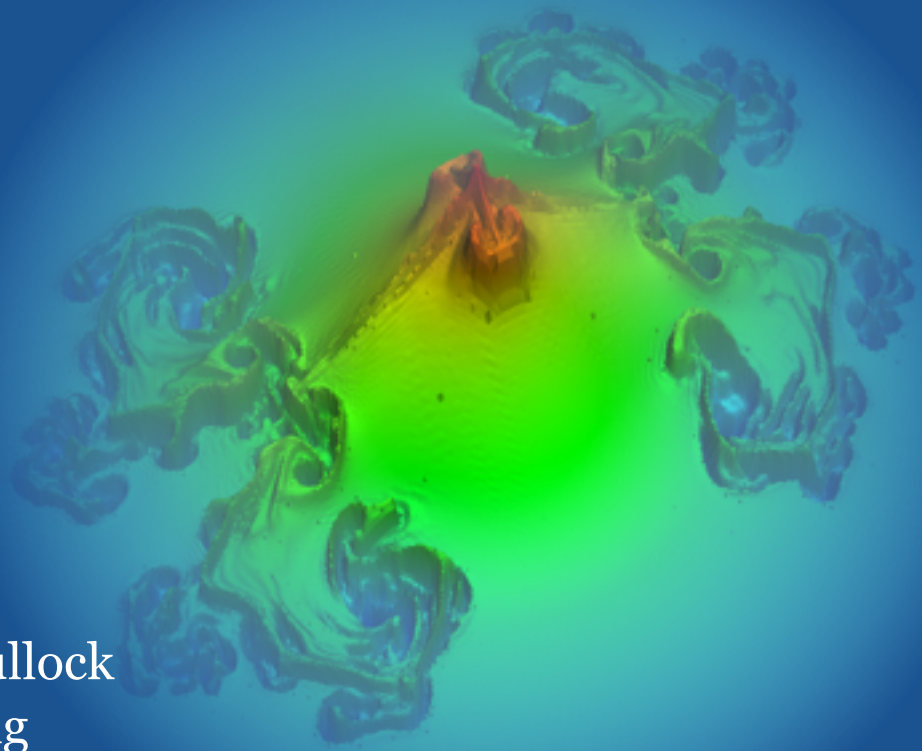


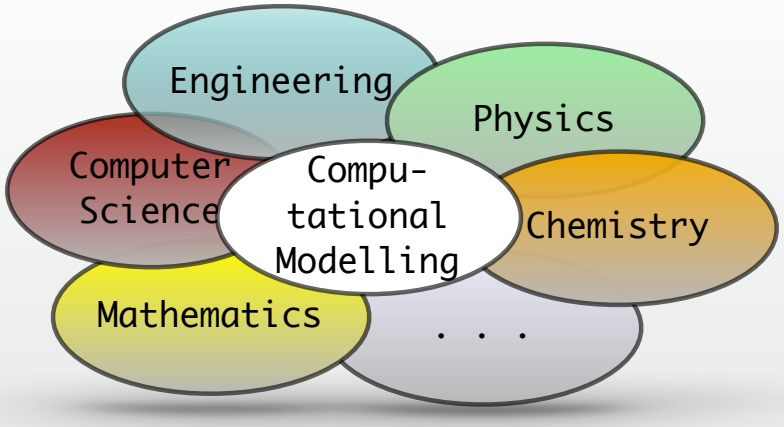
Hans Fangohr, Ian Hawke, Seth Bullock
EPSRC Centre for Doctoral Training
31 March 2014

Centre for Doctoral Training (CDT)

- New(-ish) initiative of UK research councils to improve doctoral training
- Training in cohorts of 10 – 20 students per year
- Usually
  - first year dominated by taught modules (similar to MSc), followed by
  - full-time research in years two to four
- Typically leading to PhD degree at the end of 4 years

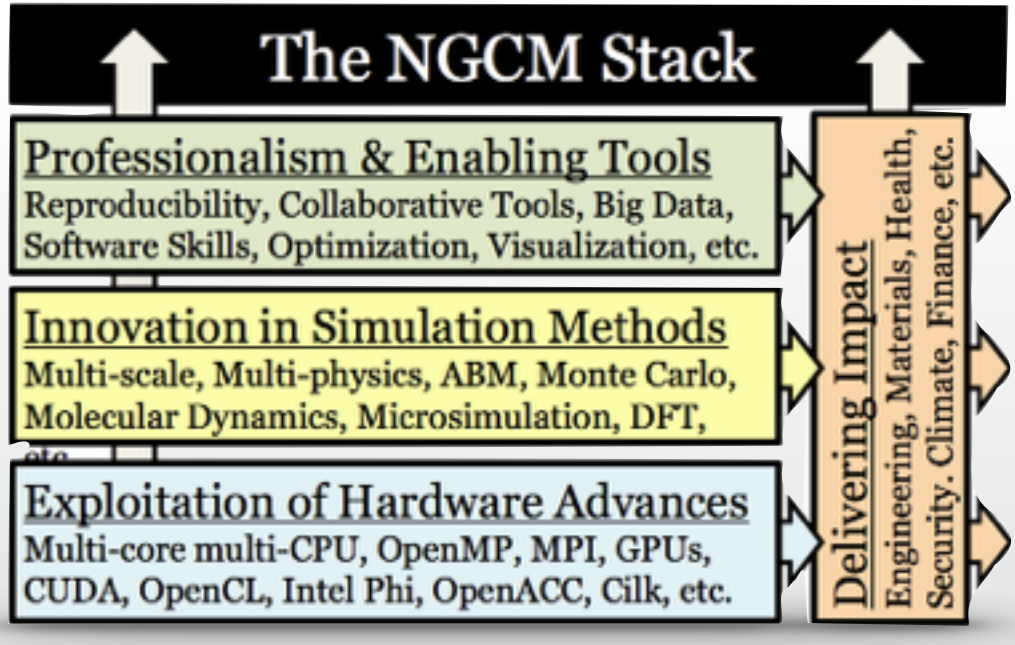
CDT in Next Generation Computational Modelling (NGCM) – why?

- 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?

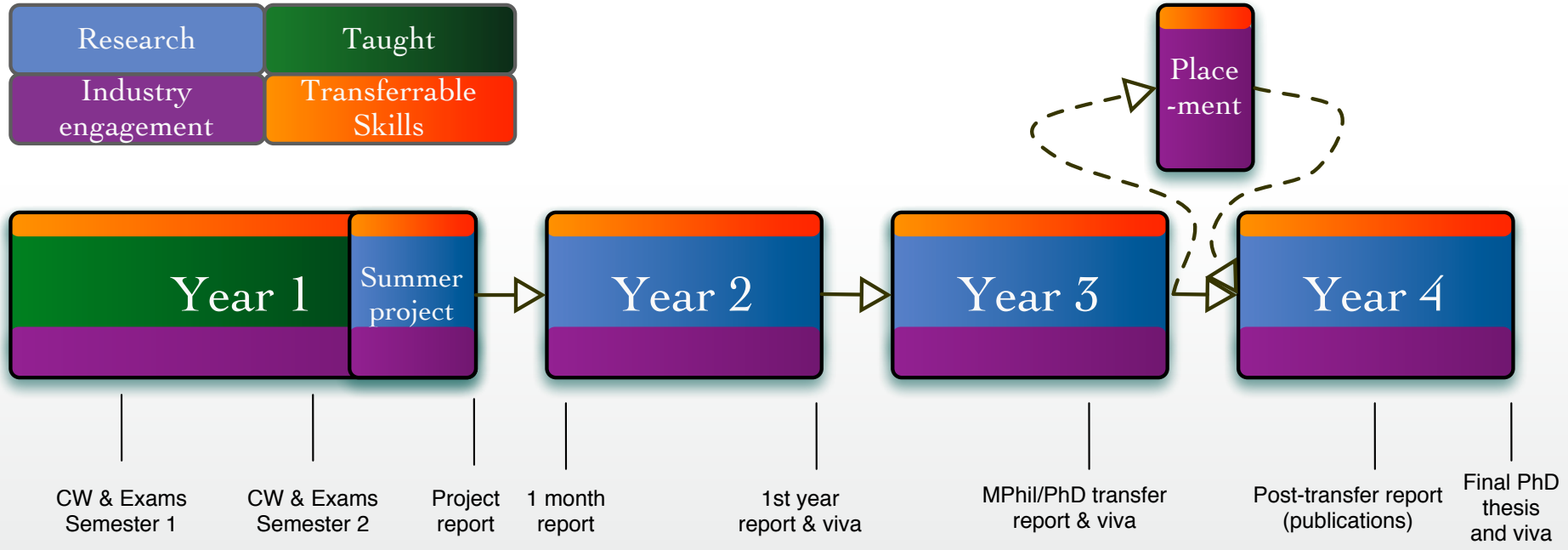
- Training and research addressing
  - professionalism
  - simulation methods
  - exploitation of latest hardware



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



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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)

Semester 1, 60 credits	**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	**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		

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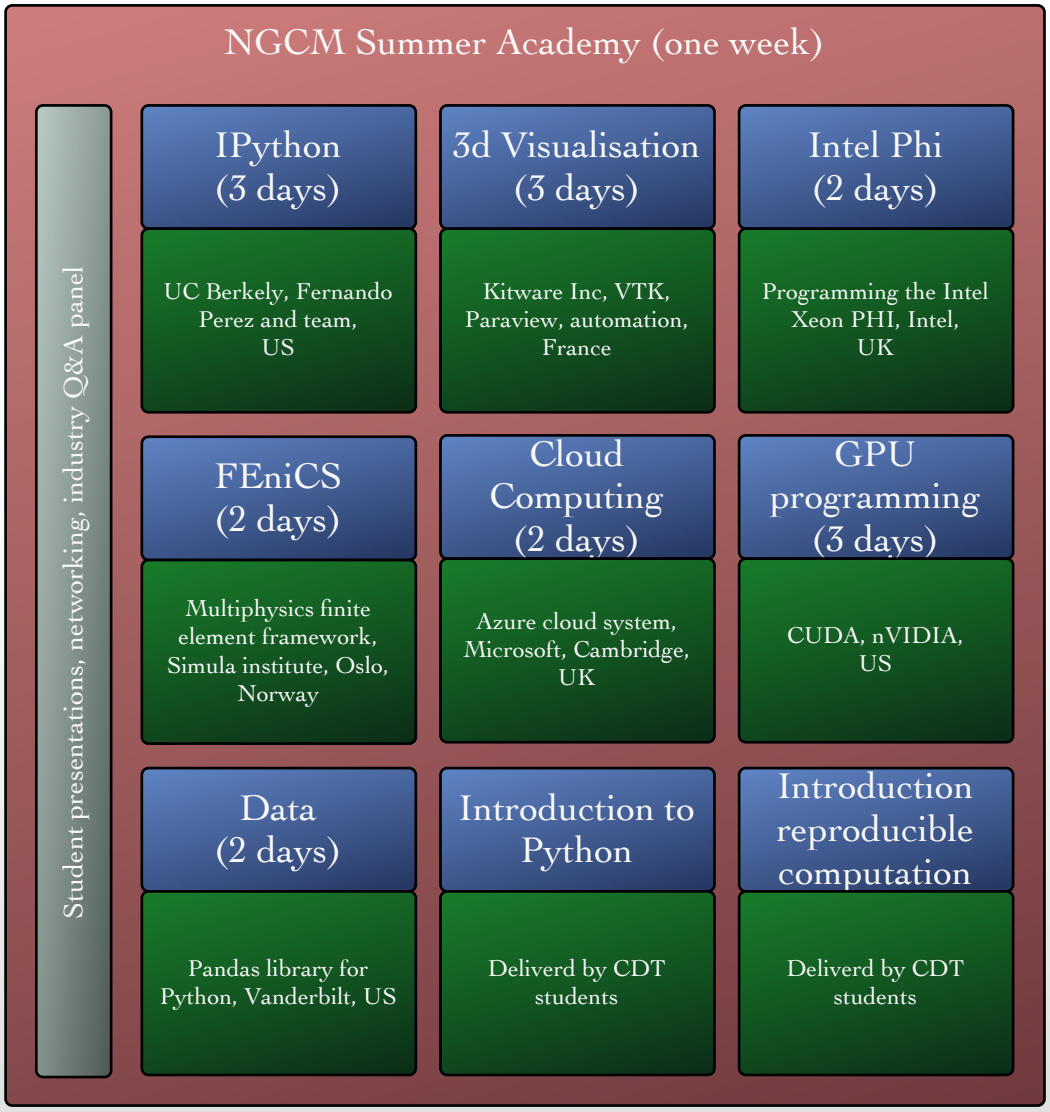
Summer Academy

- 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



Facilities:
Southampton Supercomputer Iridis

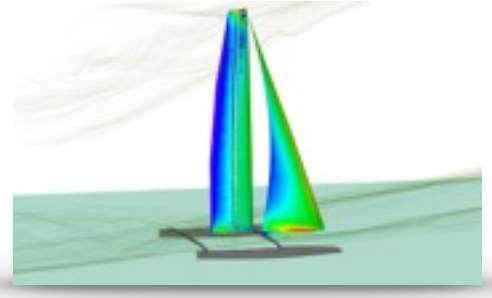
- £3.2 million investment in 2013
- hardware refresh cycle of 3 years
- part of 10-year strategy plan for High Performance Computing (HPC), i.e. long-term commitment of university

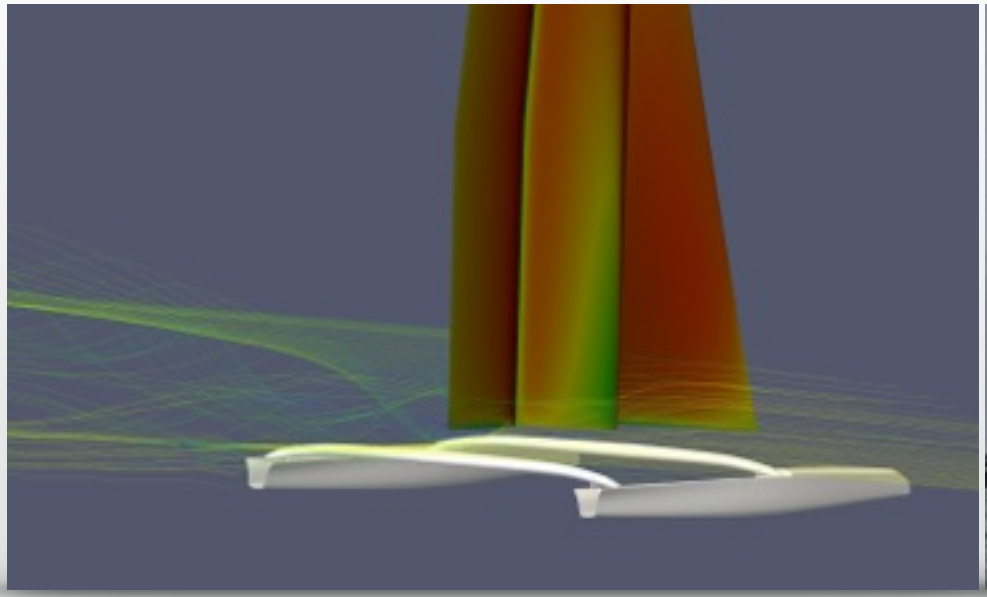
Iridis 4

- Biggest university owned computer in England
- 12200 Cores (250 TFlops);
- 16*2.6 GHz cores per node;
- 4 GB of memory per core; 64GB per node; total 49TB RAM
- 4 high-memory nodes with 256 GB of RAM;
- 24 Intel Xeon Phi Accelerators (25 TFlops);
- 1.04 PB of storage with Parallel File System;
- Infiniband network for interprocess communication

Facilities: Access to GPU cluster Emerald

- 372 NVIDIA GPUs
- 114 TF compute power
- Jointly used with Oxford, Bristol, and UCL





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

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

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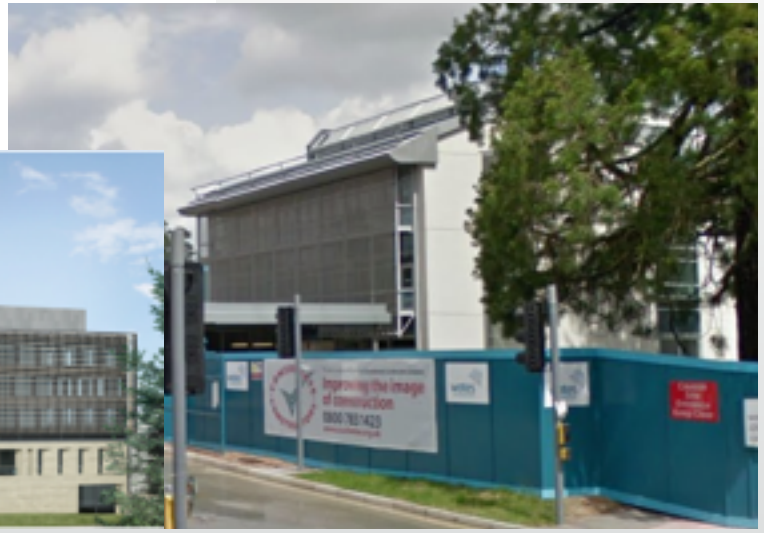
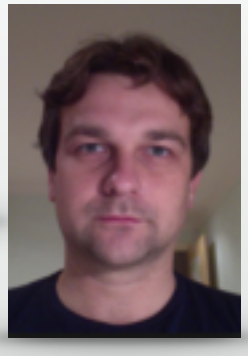
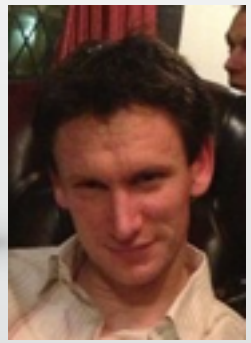


CDT Core staff

- Directors:
  - Hans Fangohr
  - Ian Hawke
  - Seth Bullock
- Tutors
  - Andras Sobester
  - Ondrej Hovorka
  - Dave Angland
- Manager (to be recruited)
- Supervisors from Computational Modelling Group

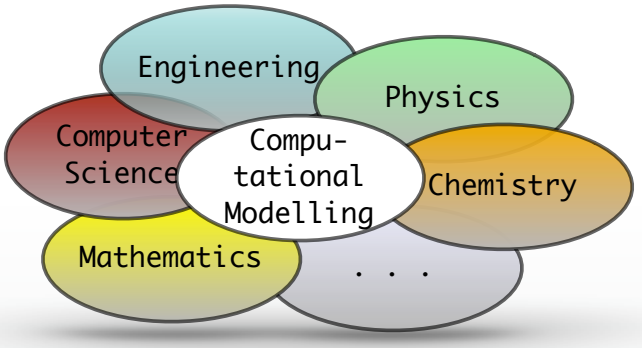




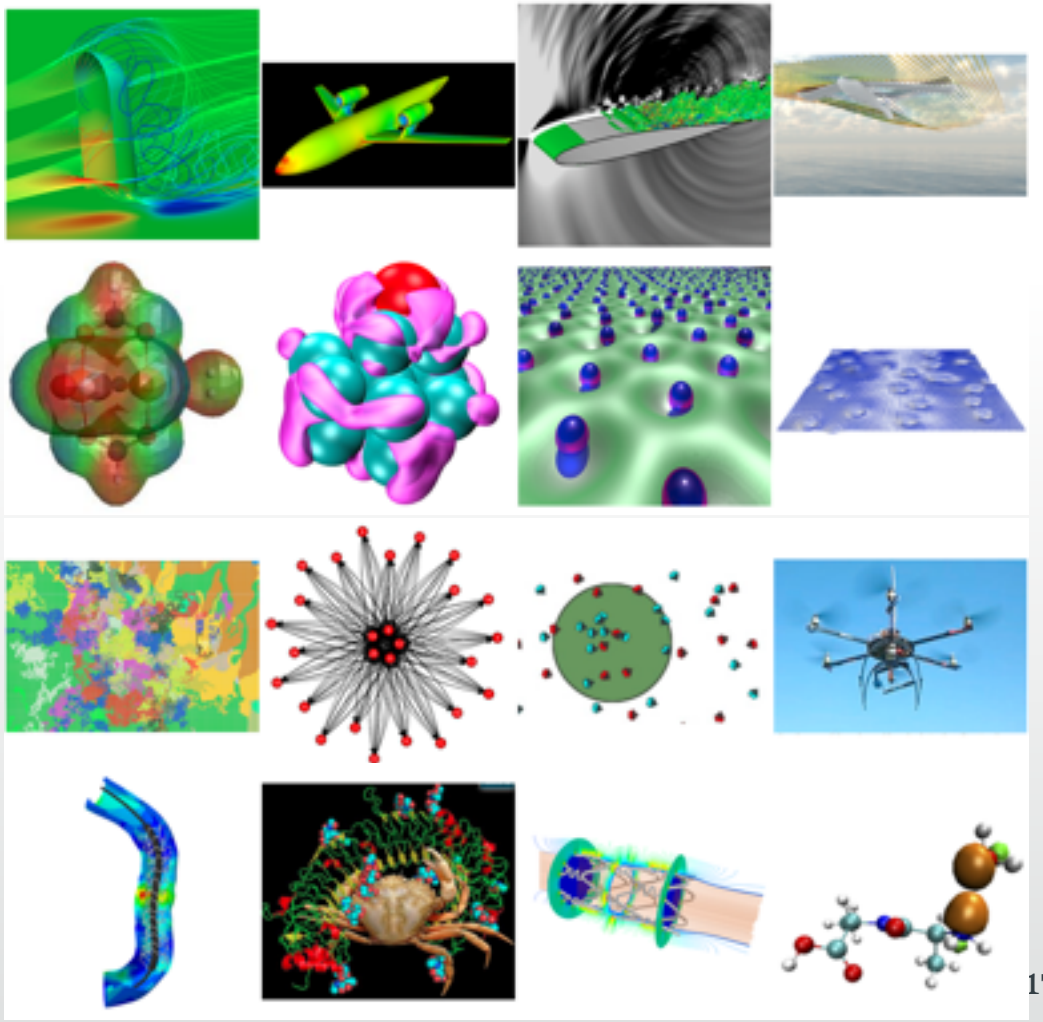
Supervisors from Computational Modelling Group

- > 170 academic staff
- > 600 post-docs and PhD
- use computer simulation to advance research and engineering
- 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



PhD projects

- will have novelty in computational method
- will have novelty in application of method

- Growing list of available projects at http://ngcm.soton.ac.uk/projects

Recruitment process

- Match academic supervisor from Southampton with industry sponsor, and outline project
- CDT to advertise projects and drive recruitment for project
- Involve sponsor in recruitment process (if desired)
- All shortlisted applicants will be interviewed
- Expect normally 1st class degree
- Studentship and studies will start Sept 2014

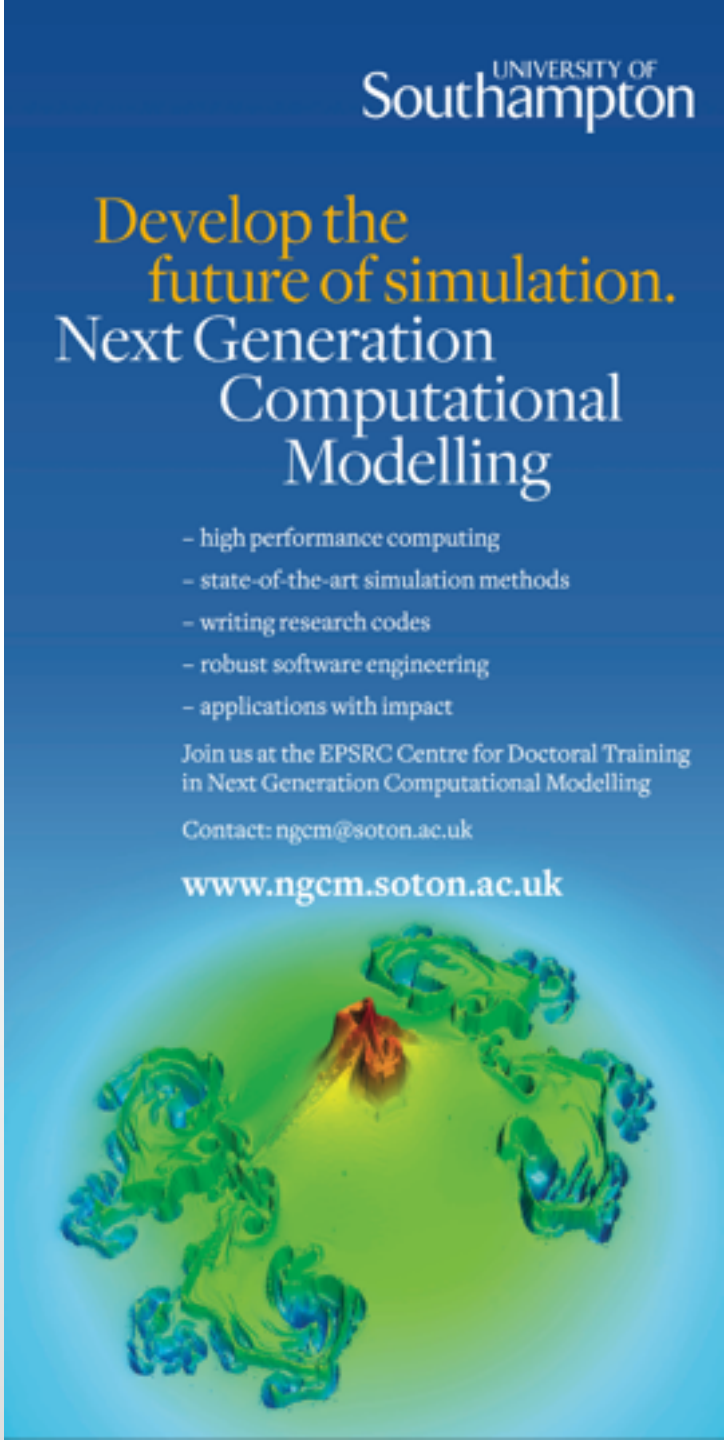
Co-funding of studentships

- Require industry contributions of (at least) £12.5k per annum over 4 years for one co-funded studentship (50% leverage provided from CDT)
- 8 of these co-funded studentships available every year
- Students engage with sponsor throughout the 4 years: familiarise with problem in semester 1 and 2, summer research project at end of year 1, then 3 years full time research on project. Placements encouraged.

CDT in Next Generation Computational Modelling

Contact

- Email: ngcm@soton.ac.uk
- Website: http://ngcm.soton.ac.uk
- Twitter: @ngcm_soton
- Phone: 023 8059 4888



IP – flexible contract

Ownership, use and protection of IP

a) All Background IP used in connection with the Studentship Project shall remain the property of the Party who introduced it.
b) Subject to clause 4f all SDRD shall be owned by the Sponsor.
c) Subject to clause 4d all Foreground IP shall belong to the University. Subject to clause 4d & 4f the University will grant the Sponsor an exclusive, royalty free, fully paid up licence (including the right to sub-license) to Foreground IP. Notwithstanding such licence the University and Student shall have the free and unfettered right to use all Foreground IP for teaching, research and development purposes without payment of any kind to the Sponsor but the University shall have no right to sub-licence Foreground IP without Sponsor's written consent.
d) The copyright of any Thesis will remain that of the Student. The University will secure a royalty free right for the Sponsor to copy and distribute the thesis for internal business purposes.
e) No licence is granted to the University's Background IP unless specifically agreed to in writing. Any existing Background IP which belongs to the University and is used in the Studentship Project will remain the property of the University. Where Background IP is necessary for use of the Foreground IP, and the University has the right to do so, the University will be willing to negotiate a non-exclusive licence with the Sponsor for rights to use such Background IP on fair and reasonable terms.
f) Ownership of SDRD and licences to Sponsor of Foreground IP and the right to negotiate a licence to Background IP shall not come into force until full payment for the Studentship Project has been received by the University and the Sponsor will not have the right to use, dispose of or in any way deal with such Foreground IP or SDRD until such time as payment has been made.
g) Upon request by the Sponsor the University shall seek patent or other registered protection for the Foreground IP at the Sponsor's expense. The University shall control and direct the patent application but shall fully consult the Sponsor and not unreasonably refuse to incorporate its wishes in any application to be made.