Computational
Modelling Group

UNIVERSITY OF
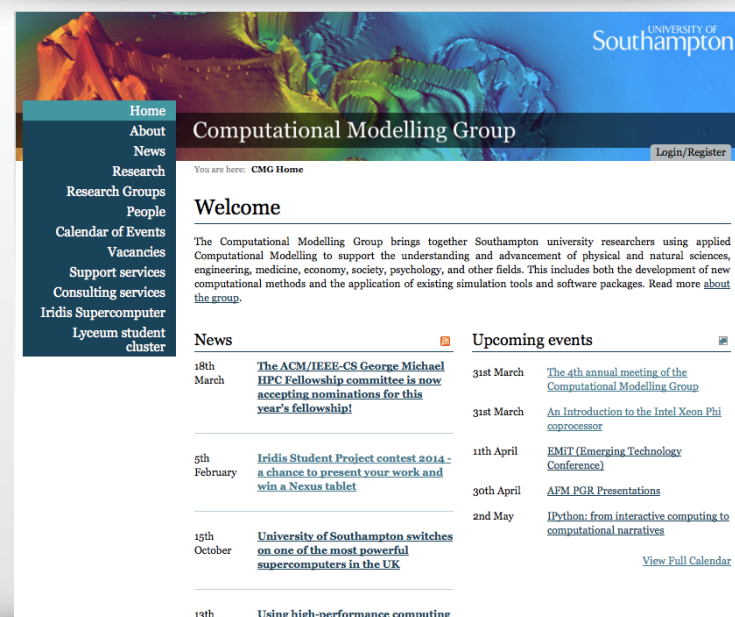Southampton

4th annual meeting
Computational Modelling Group
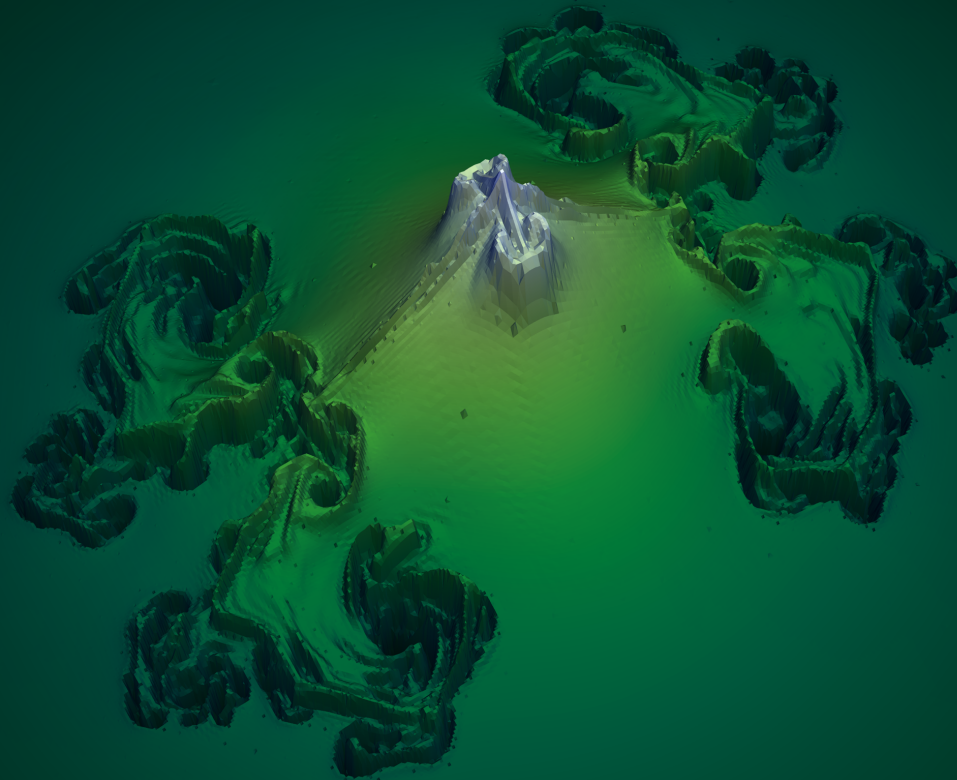
Monday 31 March 2014, http://cmg.soton.ac.uk

Outline

- History CMG

- News

  - Centre for Doctoral Training

  - Research Software Engineers

 - IPython seminar

- Today

History CMG

- Ambition to bring together all computational modelling from across university, started 2009

  - ~170 academic staff

  - ~500 PhD students and postdocs

  - ~700 events since 2009

  - ~270 projects

- joint use of Iridis supercomputer

- but also desktop computing

Centre for Doctoral Training (CDT) in Next Generation Computational Modelling (NGCM)

- £10m centre (EPSRC, industry, Uni Southampton)

- To recruit ~15 students every year (for 5 cohorts)

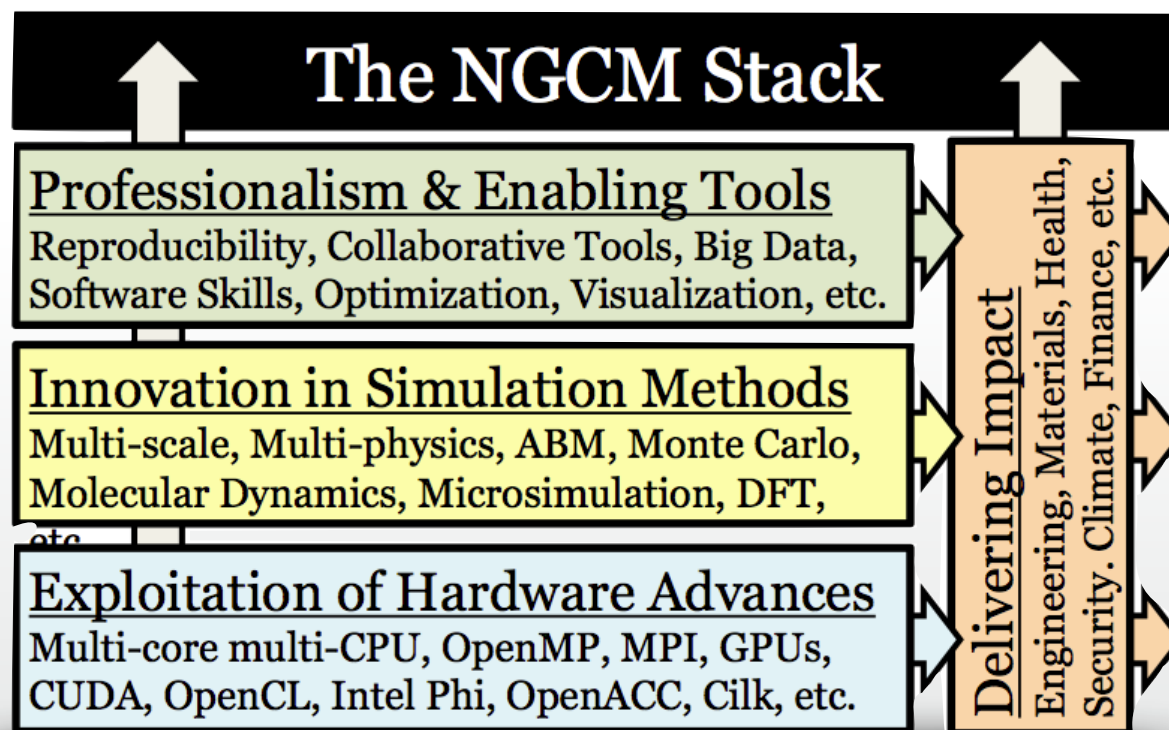- each student: 1 (mostly) taught year + 3 year research PhD
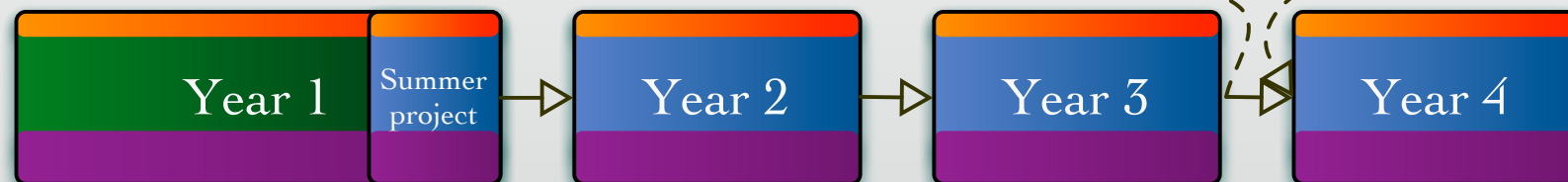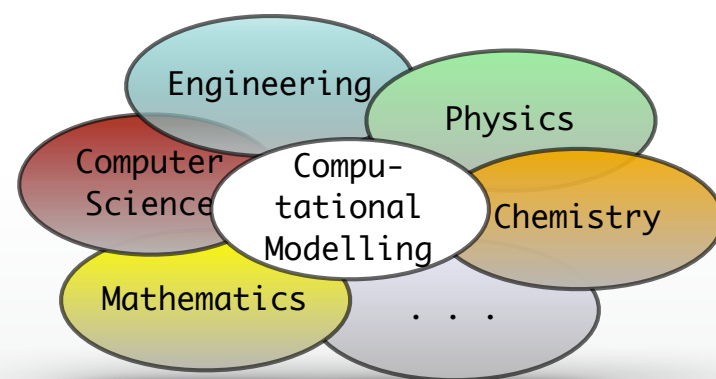
CDT in NGCM

- 8 studentships co-funded with industry

- 7 fully funded
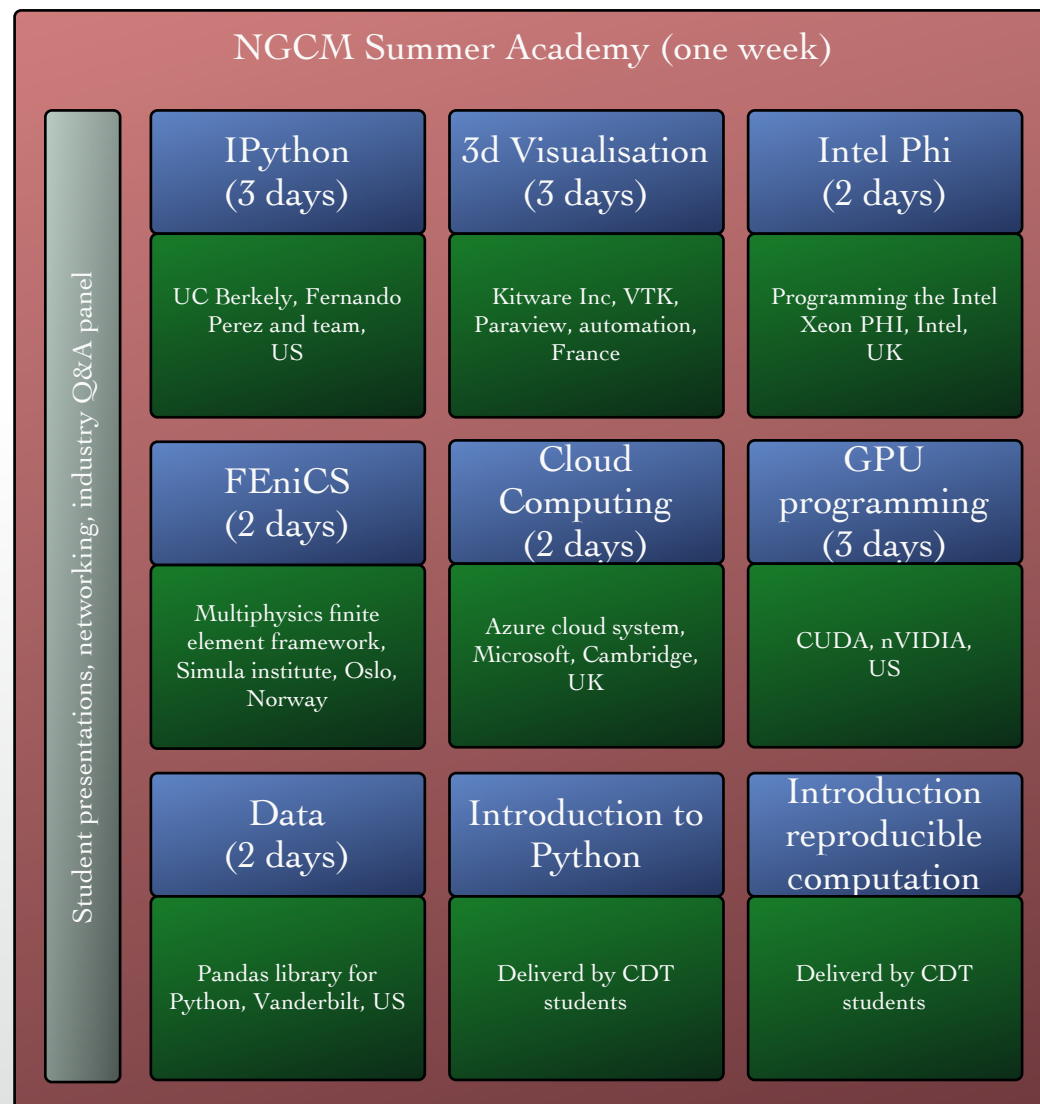
- Broad range of industrial partners

What is the NGCM focus?

The NGCM Stack

Professionalism & Enabling Tools
Reproducibility, Collaborative Tools, Big Data, Software Skills, Optimization, Visualization, etc.

Innovation in Simulation Methods
Multi-scale, Multi-physics, ABM, Monte Carlo, Molecular Dynamics, Microsimulation, DFT, etc.

Exploitation of Hardware Advances
Multi-core multi-CPU, OpenMP, MPI, GPUs, CUDA, OpenCL, Intel Phi, OpenACC, Cilk, etc.

Delivering Impact
Engineering, Materials, Health, Security. Climate, Finance, etc.

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NGCM Summer Academy

- Annual meeting from summer 2015 onwards

- Open for participation from outside Southampton

- Parallel training sessions (examples on the right)

- High Profile trainers

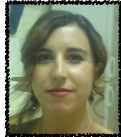- Centre of gravity for computational modelling in the UK

NGCM Summer Academy (one week)

Student presentations, networking, industry Q&A panel

IPython (3 days)
UC Berkely, Fernando Perez and team, US

3d Visualisation (3 days)
Kitware Inc, VTK, Paraview, automation, France

Intel Phi (2 days)
Programming the Intel Xeon PHI, Intel, UK

FEniCS (2 days)
Multiphysics finite element framework, Simula institute, Oslo, Norway

Cloud Computing (2 days)
Azure cloud system, Microsoft, Cambridge, UK

GPU programming (3 days)
CUDA, nVIDIA, US

Data (2 days)
Pandas library for Python, Vanderbilt, US

Introduction to Python
Deliverd by CDT students

Introduction reproducible computation
Deliverd by CDT students

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IPython Notebook seminar

- NGCM seminar

- Friday
2 May 2013, 10am

- Fernando Perez (Berkeley, CA, US)

- subscribe to
ngcm-events@lists.soton.ac.uk
for further NGCM seminars
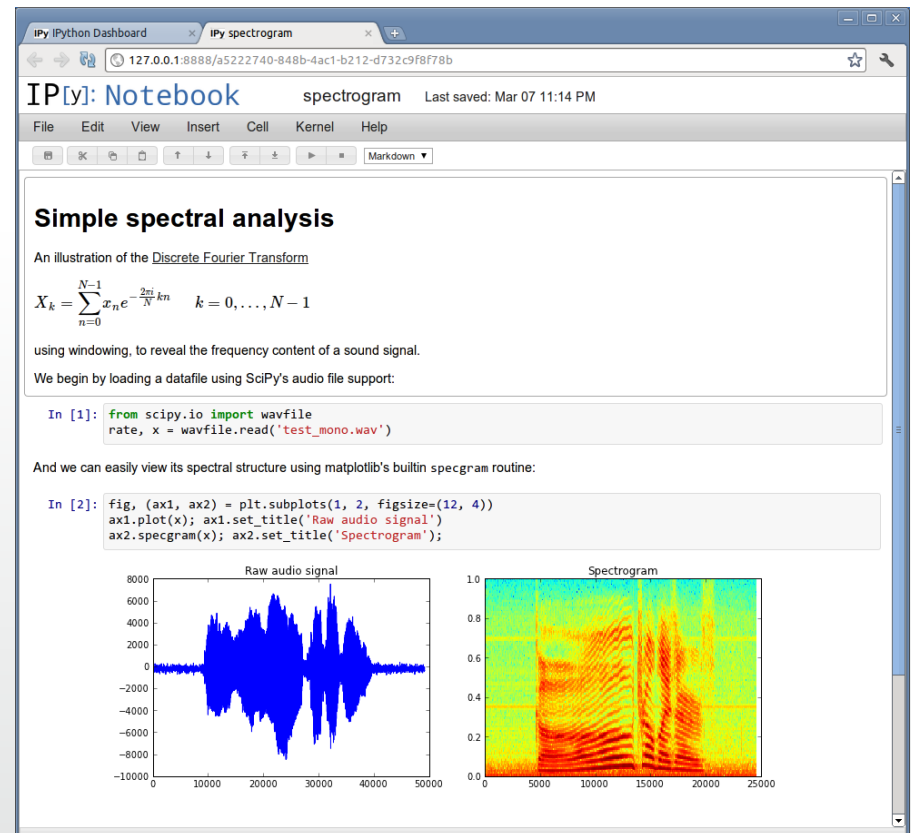
NGCM Summary and contact

- General info: www.ngcm.soton.ac.uk

- Twitter: @NGCM_Soton

- Email: ngcm@soton.ac.uk

- NGCM Seminar announcements etc:
  ngcm-events@lists.soton.ac.uk

Programme today

- 11:20 PhD student Iridis project competition
  - 11:25 Alicia Costalago Meruelo
  - 11:40 Georgios Ragkousis
  - 11:55 Robin Wilson
- 12:10 Oz Parchment: Arrival of Iridis 4
- 12:20 Jess Jones: Xeon Phis – first impressions
- 12:45 Announcement of competition winner (ProVC Petts)
- *13:00 Lunch, posters, PhD projects, networking*
- 14:00 NGCM Open Day: Q & A with directors, DTC students (LT B)
- 14:00 Intel Workshop on Intel Phi (LT A)