

# ***HPC for Scientific Computing***

***Dr Matt Ismail***  
***Centre for Scientific Computing***

# Talk overview

- Introduction to CSC
- HPC kit
- “Francesca 2”

# CSC: an interdisciplinary research centre

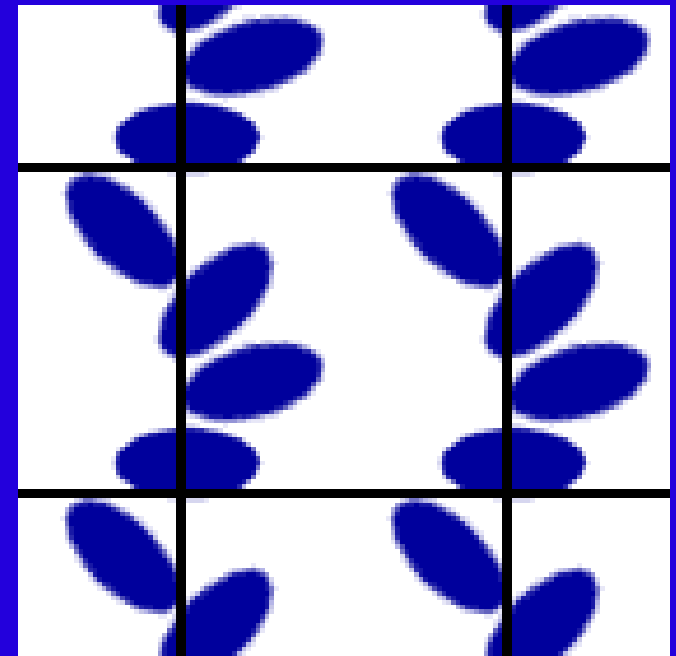
- nurtures computationally-driven research
- national teaching and training centre
- provides a HPC service

# CSC as a research centre

- Core research
  - fundamentals
  - molecular dynamics and modelling
  - computational engineering and fluids
  - Monte Carlo and stochastic simulation
  - quantum simulations
  - computation of living systems
- 20 core academic staff from 7 departments

# Molecular Dynamics and Modelling

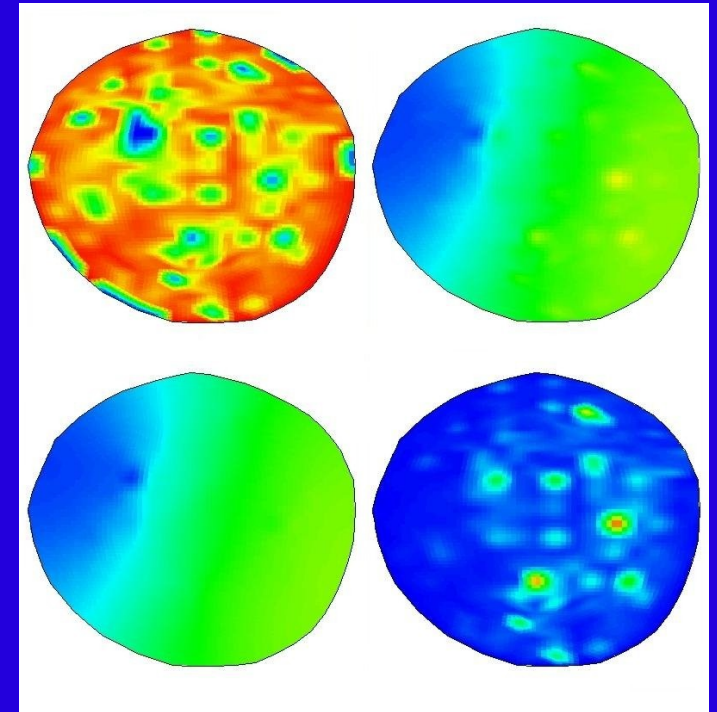
- MD concerns particle motion inherent to natural processes such as molecular vibration or bond stretching and bending
- Disciplines include Chemistry, Physics and Mathematics
- Example projects are e.g. The biological interface with materials or differential equations with random initial data



Periodic boundaries for molecular simulations

# Computational Systems Biology

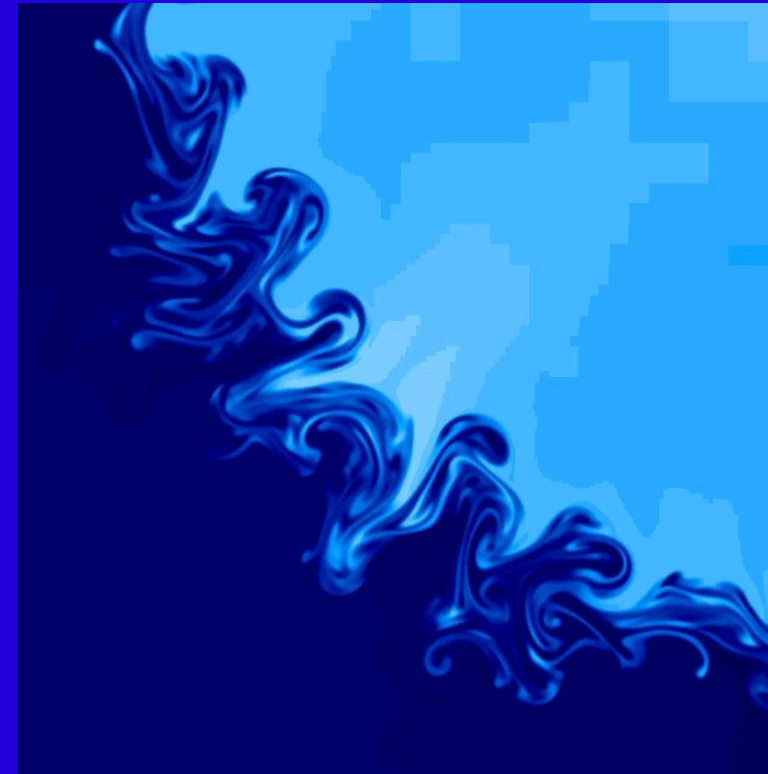
- Systems biology studies complexity in biological systems e.g. gene expression, cell signalling or biological image analysis
- Disciplines include Mathematics, Computer Science, Physics
- Example projects are electronic transport in DNA and molecular simulation and modelling in the life sciences



Transport and reaction  
simulation in cells

# Computational Fluid Dynamics


- CFD concerns the simulation of fluid flow usually in the presence of some complication such as e.g. turbulence, chemical reaction or mass transfer
- Physics, Mathematics and Engineering
- Example projects include simulation of magnetohydrodynamics (MHD) and turbulence simulation




Adaptive mesh high resolution  
image of Rayleigh-Taylor  
unstable flows

# Teaching and Training

- National EPSRC Training Centre
- Taught MSc in Scientific Computing
  - High Performance Scientific Computing
  - Computational Linear Algebra and Optimisation
  - Data structure and algorithms
  - Monte Carlo Methods
  - Computational PDEs
- MSc by research or PhD in Scientific Computing




MSc & PhD Degrees  
**Centre for Scientific Computing**  
Molecular Dynamics and Modelling  
Monte Carlo Methods  
Computational PDEs  
Quantum Simulations  
Computational Fluid Dynamics  
Computational Systems Biology



Underlying the research goals of the Centre for Scientific Computing (CSC) is a graduate level educational and training program including a taught MSc in Scientific Computing, as well as research programs at both the PhD and MSc level. The taught MSc course is part of an EPSRC-funded Training Centre in High-End Computing. Students will work a state-of-the-art High-Performance Computing environment throughout the course. The CSC is built around a core of researchers from several Science Departments and fosters collaborative and interdisciplinary research across the whole University.

Centre for Scientific Computing, University of Warwick,  
Gibbet Hill Road, Coventry, CV4 7AL, UK  
Phone: +44 (0) 2476 751111 Fax: +44 (0) 2476 757123  
E-mail: [csc-admissions@warwick.ac.uk](mailto:csc-admissions@warwick.ac.uk)

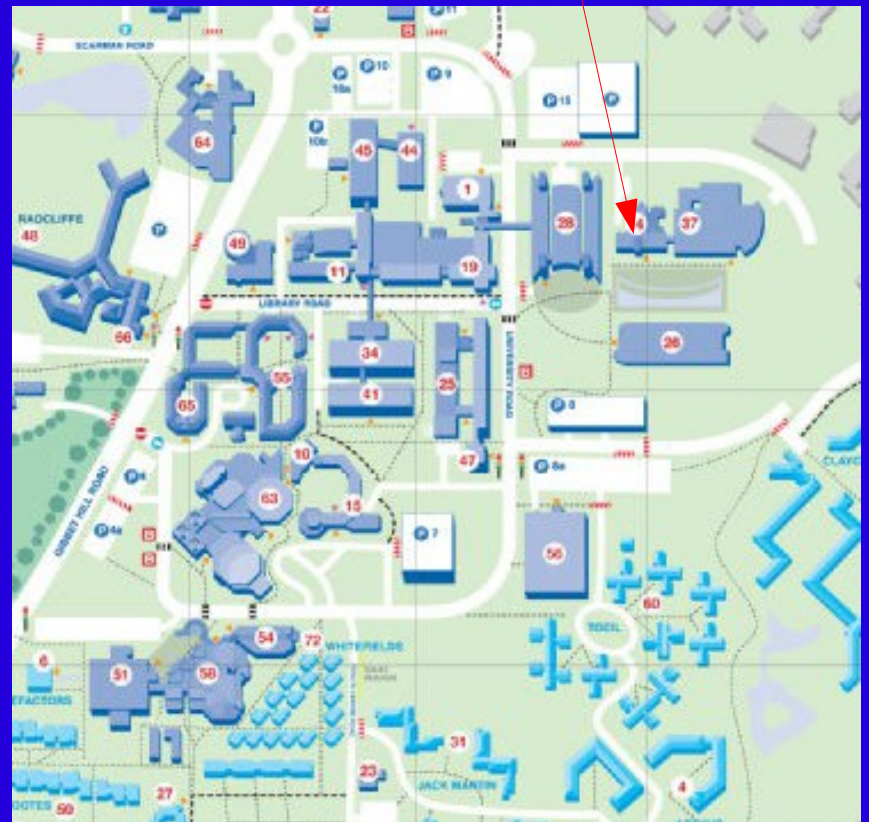


[www.warwick.ac.uk/go/CSC](http://www.warwick.ac.uk/go/CSC)



# Interacting with CSC

- CSC@Lunch
  - Mondays, 13:00 – 14:00
- Coffee and Cookies
  - Fridays, 14:00 – 15:00



# Talk overview

- Introduction to CSC
- HPC kit
- “Francesca 2”

# Branscomb Pyramid<sup>1</sup>

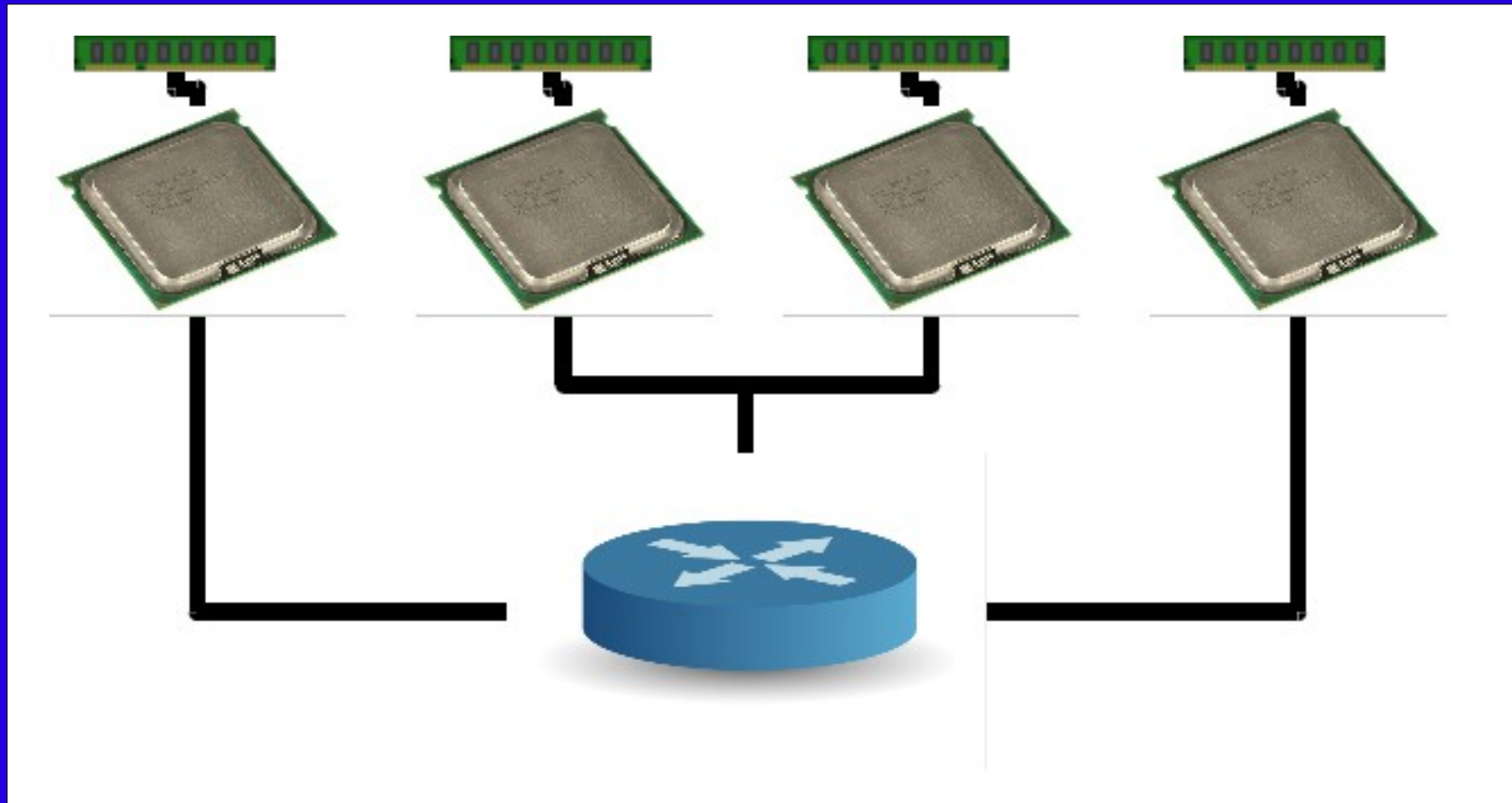


<sup>1</sup>International Review of Research Using HPC in the UK, December 2005, EPSRC

# HPC kit

- Three HPC environments
  - Distributed memory cluster for parallel computing
  - Shared memory machine (SMP)
  - Cluster of Workstations for task farming

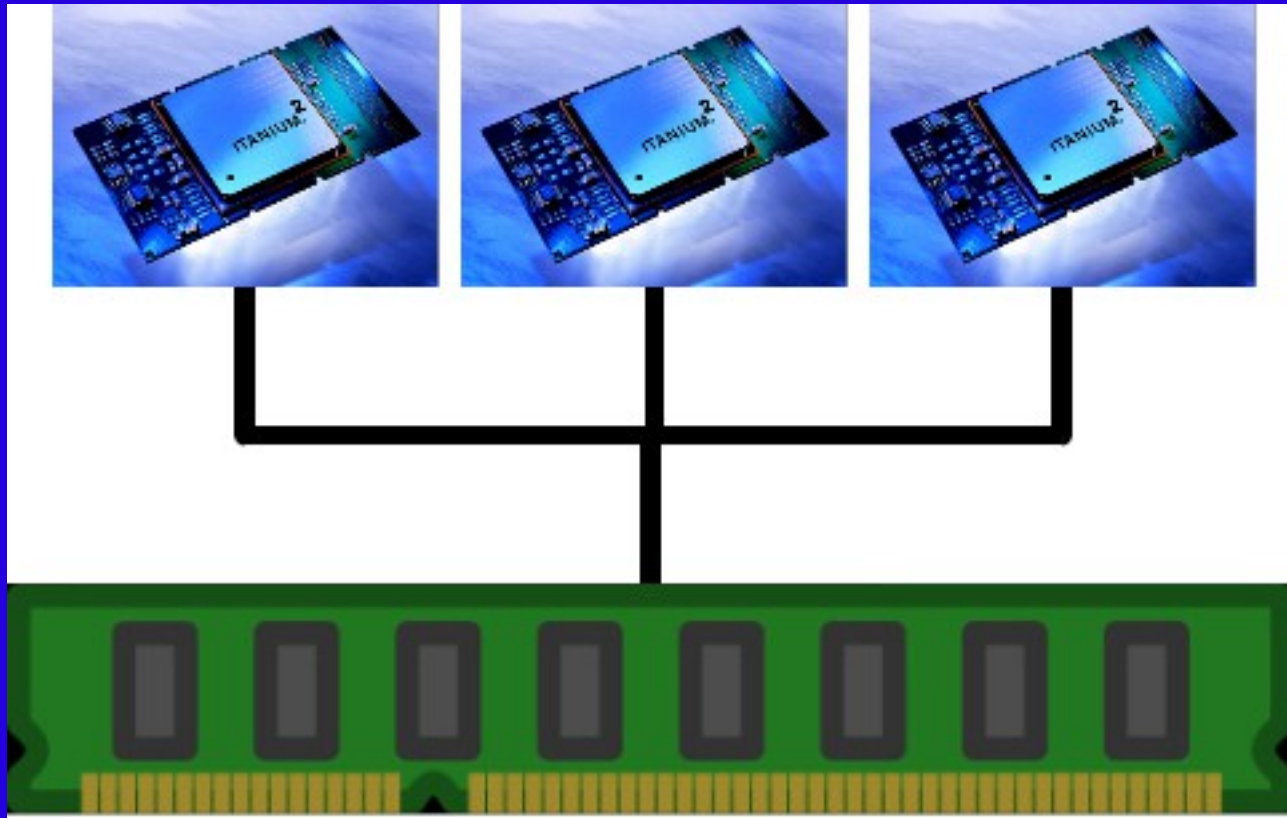
# Distributed Memory Cluster



# Distributed Memory Cluster

- “Francesca” installed 2007
  - 960 Intel “Woodcrest” 3GHz cores / 1.92 TB RAM / low latency InfiniBand / Linux / water-cooled / GPFS parallel file system
  - now end of life
- “Francesca 2” installed December 2010
  - successor to “Francesca”

# SMP

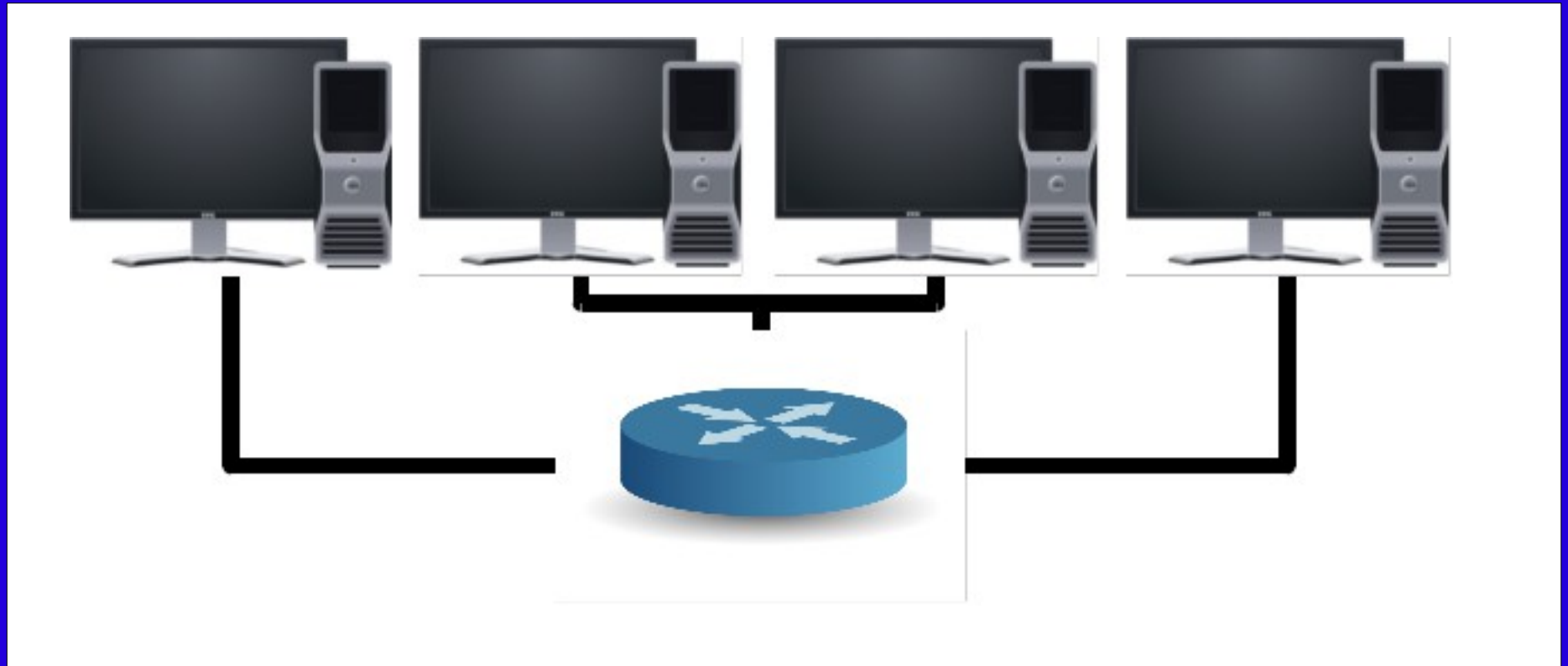


# SMP

- “skua” installed December 2004
  - SGI Altix
  - 56-way single system image / 112GB RAM / Intel Itanium2 1.6 GHz processors / Linux
  - now reached end of life
- “Francesca 2” will have SMP component



# Cluster of Workstations



# Cluster of Workstations

- Intended for Task Farming
- Layered on top of Linux workstations
- Utilises “free” CPU cycles for computation
- ~700 heterogeneous cores

# Architecture Comparison

- Distributed memory cluster
  - harder to program for because of need to use MPI
  - scalable and portable
  - Commodity clusters are cost effective
- SMP
  - OpenMP easier and compiler can do some of the work
  - less scalable and less portable than MPI
  - SMP machines are expensive
- COW
  - data parallel applications
  - visualization
  - code development and testing

# Talk overview

- Introduction to CSC
- HPC kit
- “Francesca 2”

# Machines past and present

2001

2002

2003

2005

2007



# Francesca 2

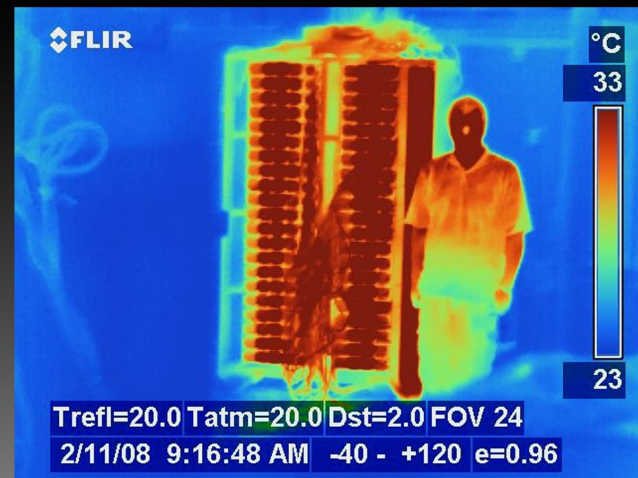
- Shared HPC facility between University and UK MHD consortium
- Delivery this month (December 2010)
- In production for research use in early 2011
- IBM system based on “iDataPlex”
- Collaboration with IBM Research

# iDataPlex

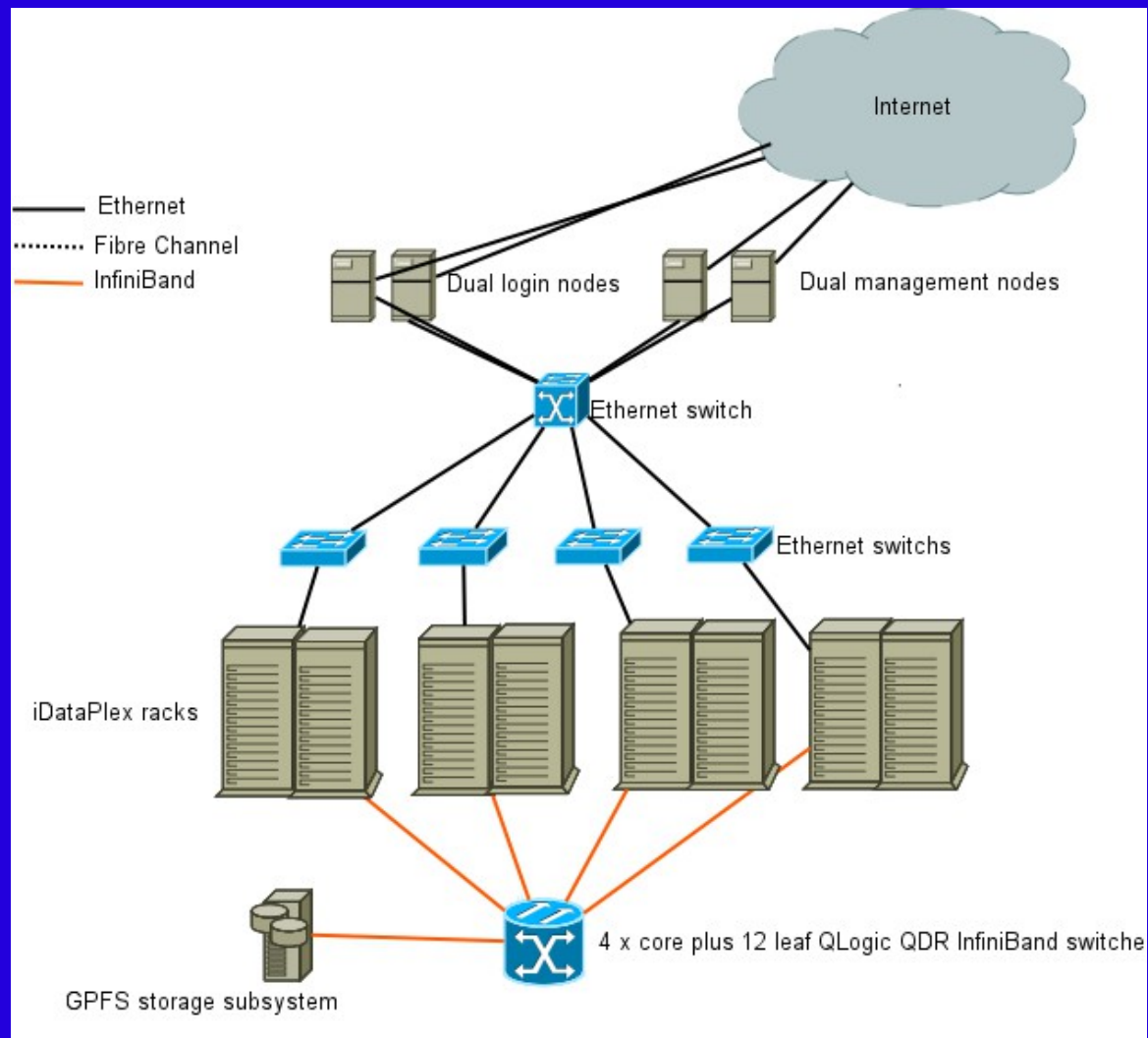


# iDataPlex

- Energy efficient design



# Francesca 2

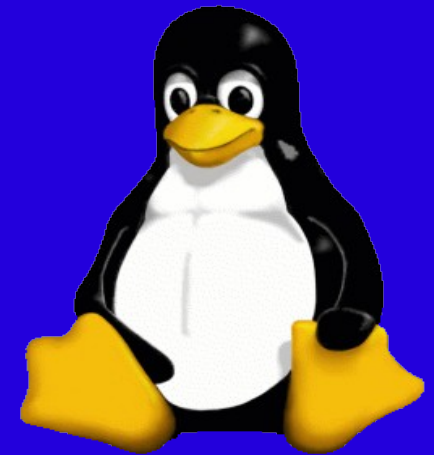


# Francesca 2

- Technical specifications
  - 2.66 GHz Intel “Westmere” hexacore processors
    - AMD “Magny-Cours” considered but slower per core
  - 265 nodes with 12 cores per node = 3180 cores
  - 33.8 TFLOPS
  - QLogic QDR InfiniBand interconnect
    - Mellanox ConnectX considered but lower MPI message rate

# Francesca 2

- Software
  - Linux OS
  - Open MPI
  - Intel Cluster Tools
  - IBM GPFS
  - MOAB/Torque
  - xCAT



# Francesca 2

- xCAT
  - “Extreme Cloud Administration Toolkit”
    - provision OS on physical or virtual machine
    - remote “lights out” management
    - open source
- MOAB
  - powerful meta-scheduler
  - can drive xCAT to provision resources on the fly
- xCAT + MOAB = adaptive computing

# Francesca 2

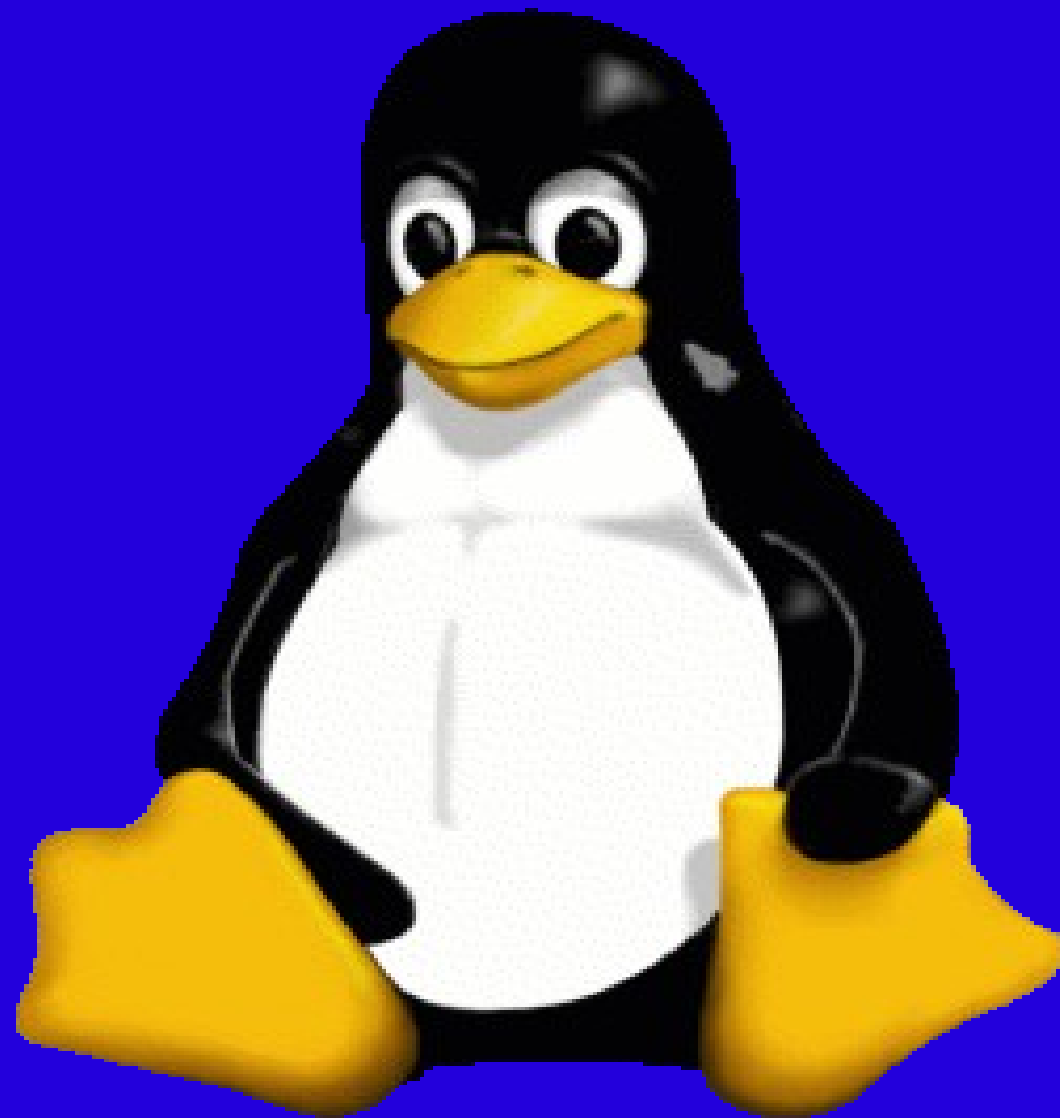
- GPU nodes
  - NVIDIA M2050 GPU Computing Modules
    - GPUs offer potential large performance gains for the right application
    - Worlds fastest supercomputer “Tianhe-1” is GPU-based
    - CUDA or OpenCL
- SMP nodes
  - Commodity nodes with large RAM
    - cost-effective alternative to dedicated SMP

# Francesca 2

- Collaborative relationship with IBM Research
  - cloud computing
    - pilot projects in cloud computing for research
    - potential application to regional HPC
    - hardware donation to kick-start the project
  - access to Blue Gene technology and expertise at IBM Watson
  - alignment with IBM's “Smarter Planet” themes

# Conclusions

- CSC is a research centre with expertise in scientific and high performance computing
- CSC supports teaching and training in scientific computing
- CSC provides substantial HPC services both nationally and locally
- Why not consider HPC or scientific computing for further study?



Centre for Scientific Computing