

HPC for Scientific Computing

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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

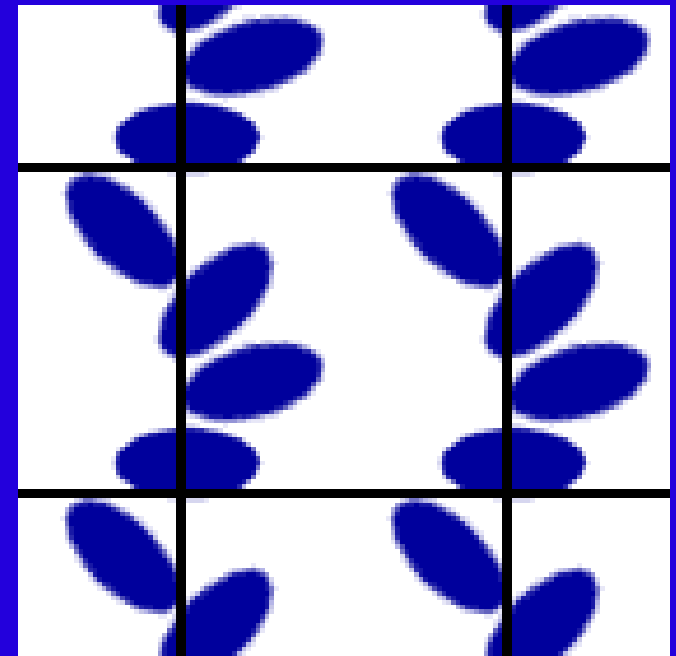
CSC as a research centre

- 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

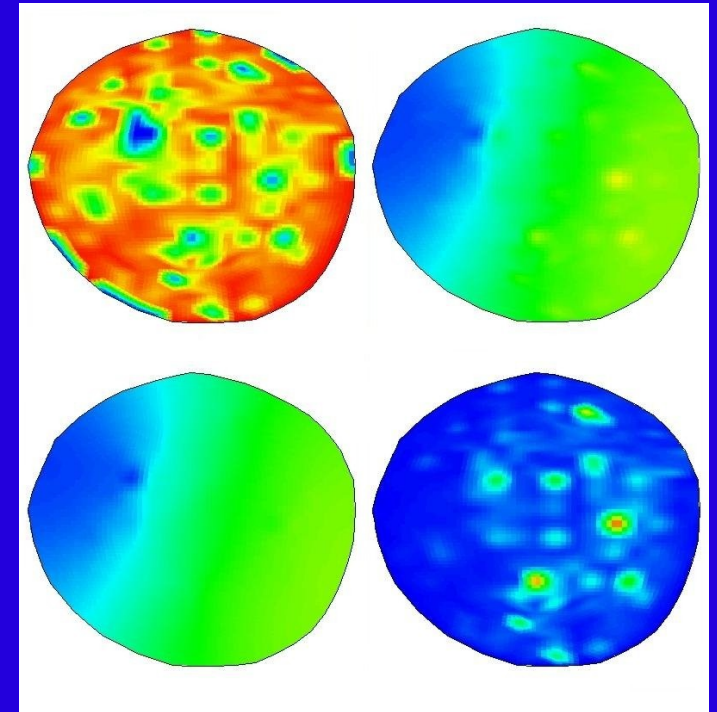
- MD concerns particle motion inherent to natural processes such as molecular vibration or bond stretching and bending
- Disciplines include Chemistry, Physics and Mathematics
- Example projects are e.g. The biological interface with materials or differential equations with random initial data



Periodic boundaries for molecular simulations

Computational Systems Biology

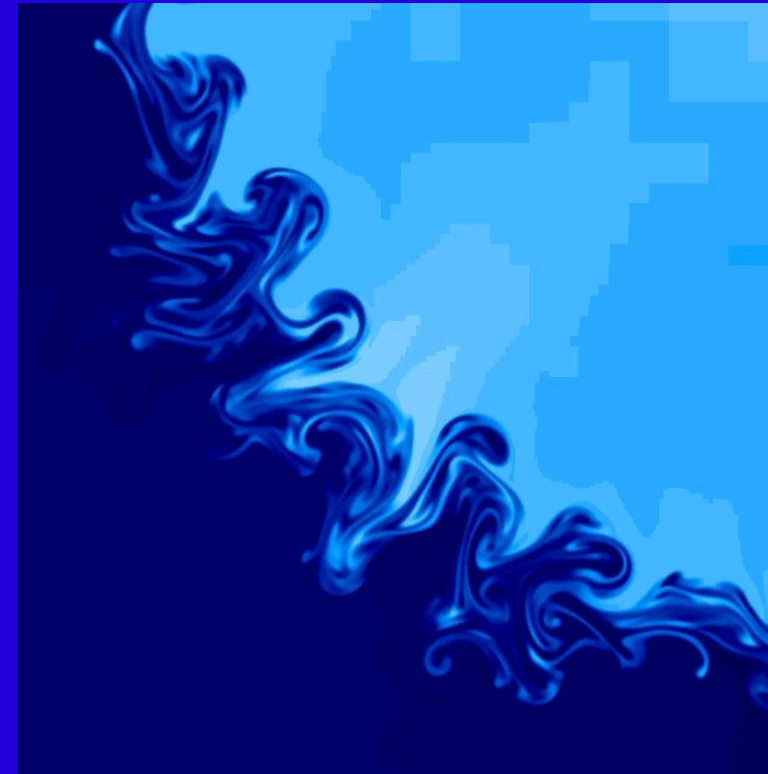
- Systems biology studies complexity in biological systems e.g. gene expression, cell signalling or biological image analysis
- Disciplines include Mathematics, Computer Science, Physics
- Example projects are electronic transport in DNA and molecular simulation and modelling in the life sciences



Transport and reaction
simulation in cells

Computational Fluid Dynamics

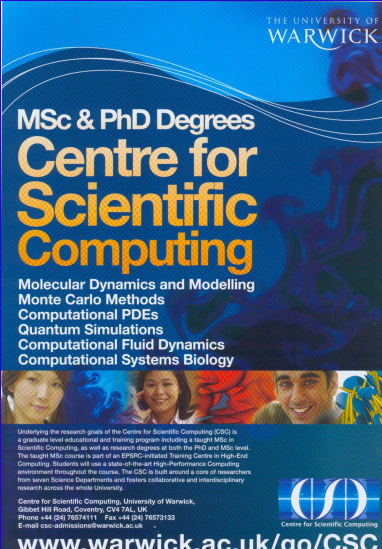
- CFD concerns the simulation of fluid flow usually in the presence of some complication such as e.g. turbulence, chemical reaction or mass transfer
- Physics, Mathematics and Engineering
- Example projects include simulation of magnetohydrodynamics (MHD) and turbulence simulation



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



THE UNIVERSITY OF
WARWICK

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.

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Interacting with CSC

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



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Branscomb Pyramid¹

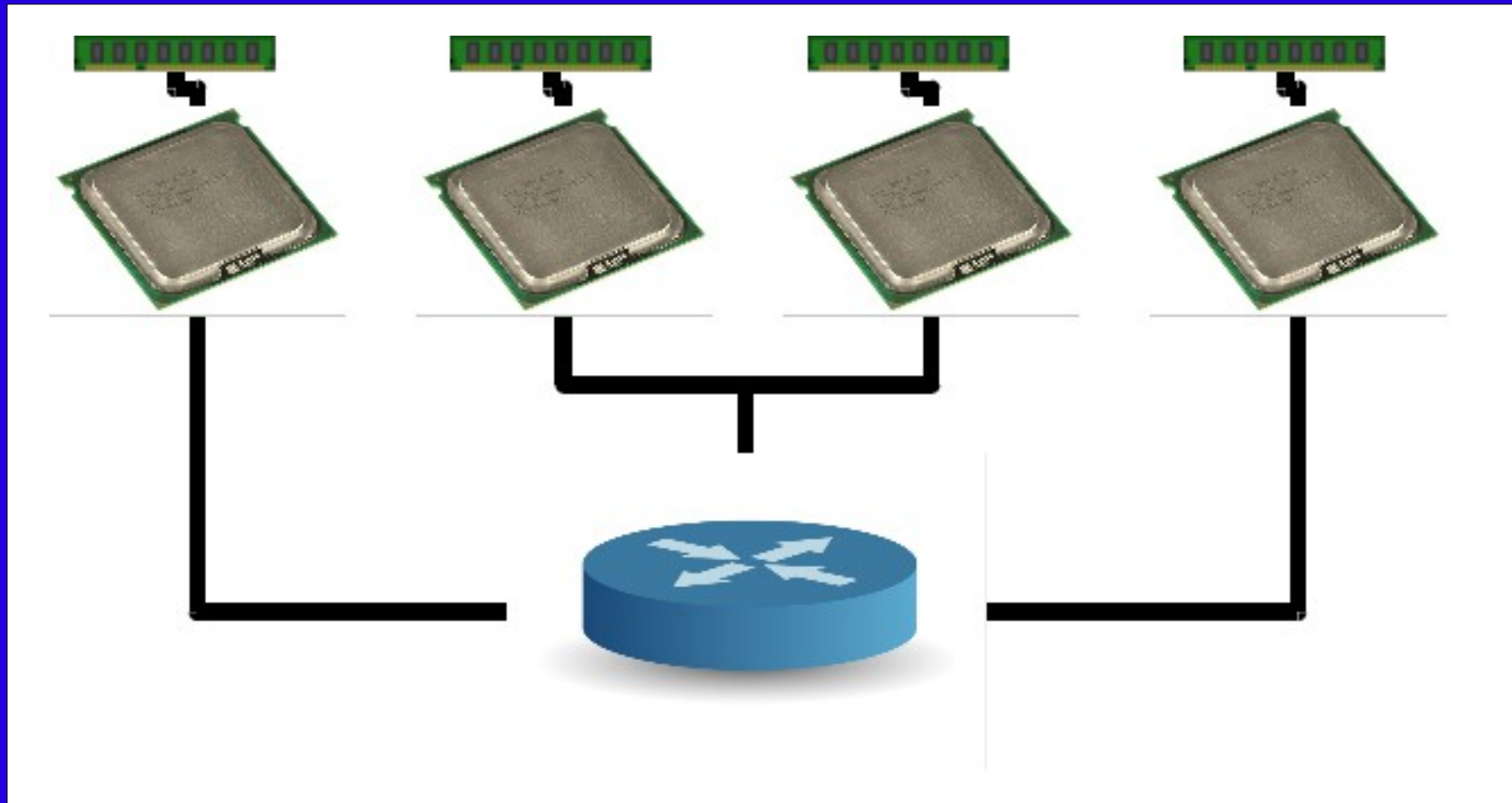


¹International Review of Research Using HPC in the UK, December 2005, EPSRC

HPC kit

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

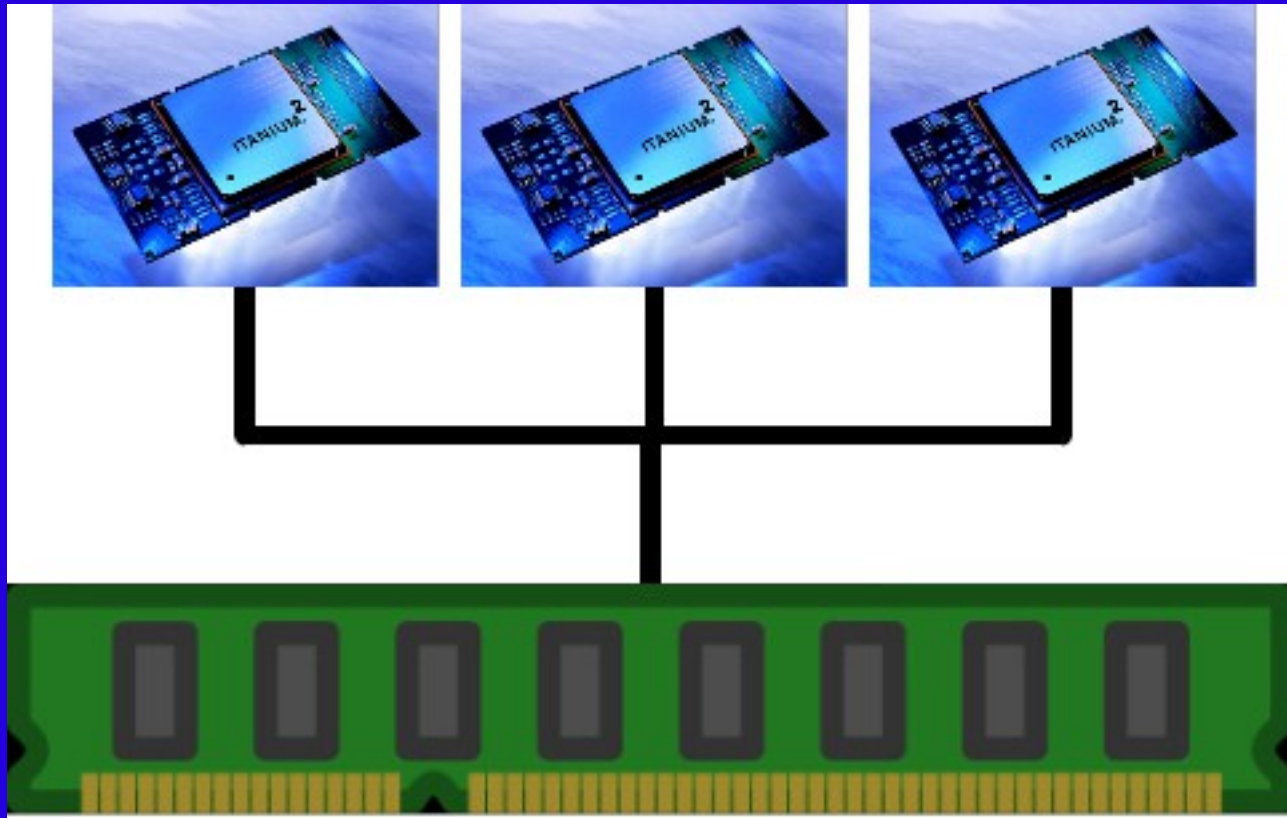
Distributed Memory Cluster



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

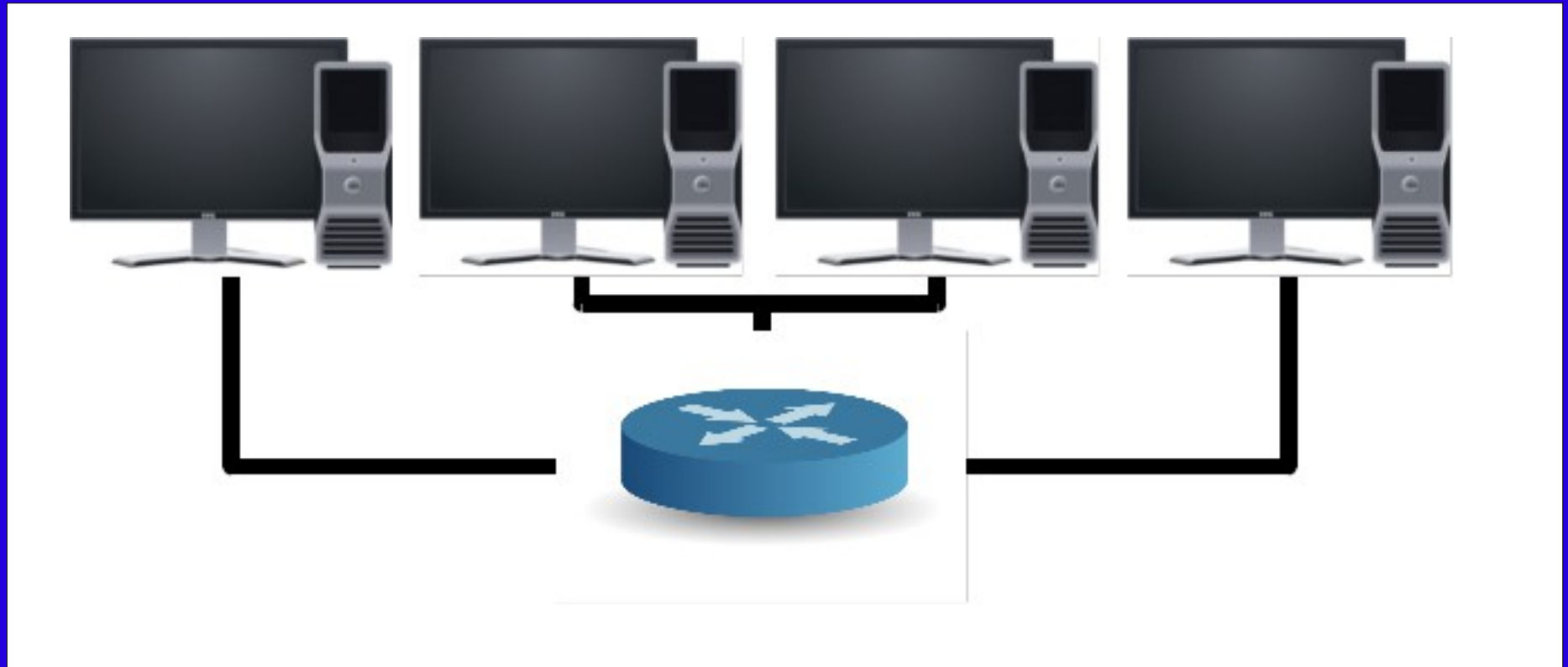


SMP

- “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

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Machines past and present

2001

2002

2003

2005

2007



Francesca 2

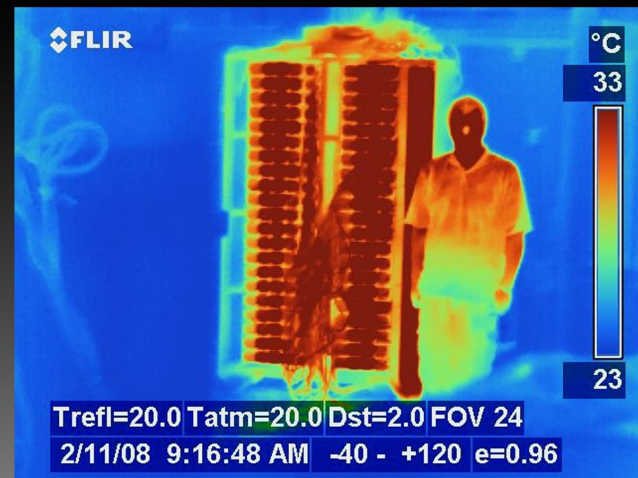
- Shared HPC facility between University and UK MHD consortium
- Delivery this month (December 2010)
- In production for research use in early 2011
- IBM system based on “iDataPlex”
- Collaboration with IBM Research

iDataPlex

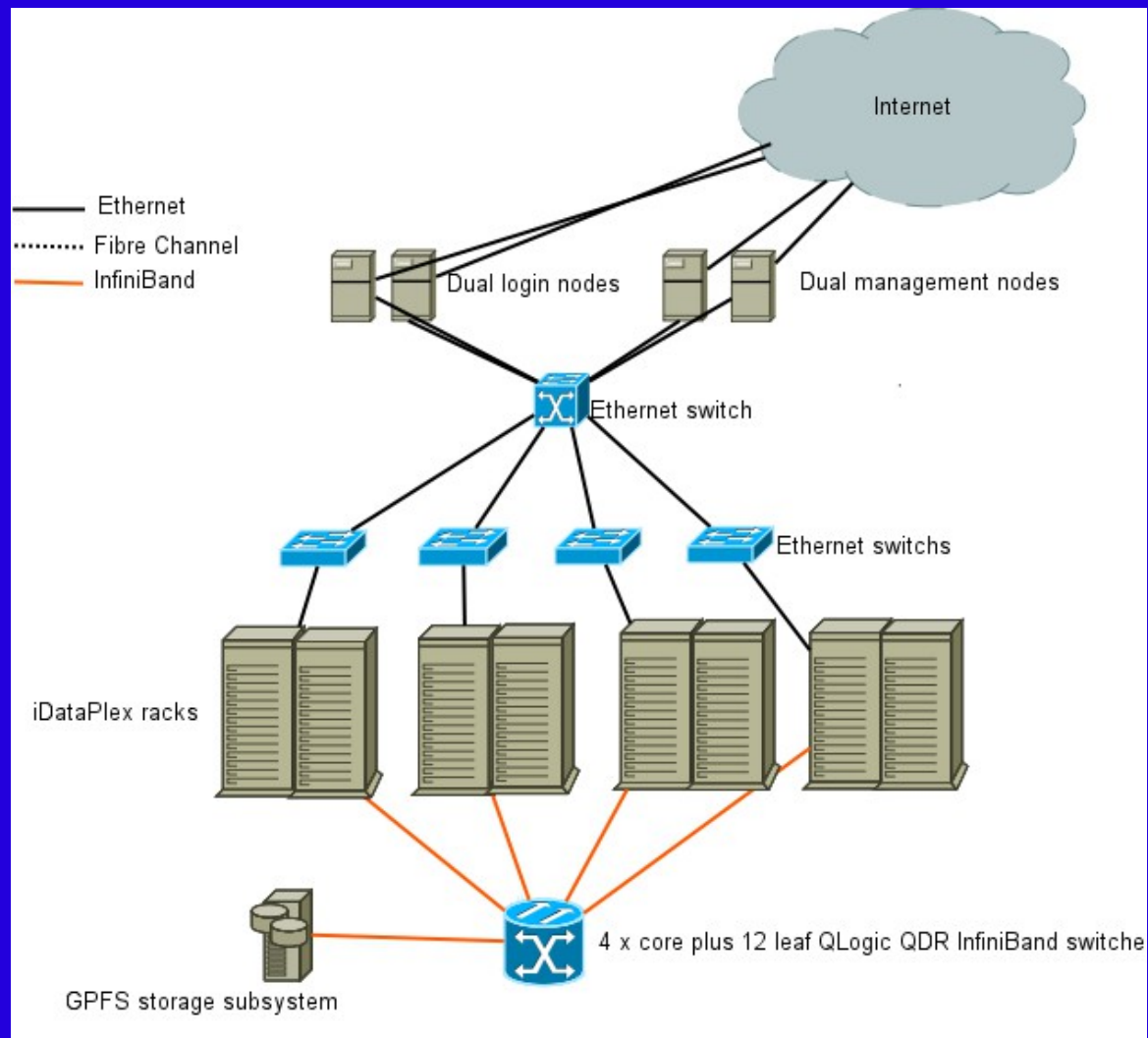


iDataPlex

- Energy efficient design



Francesca 2

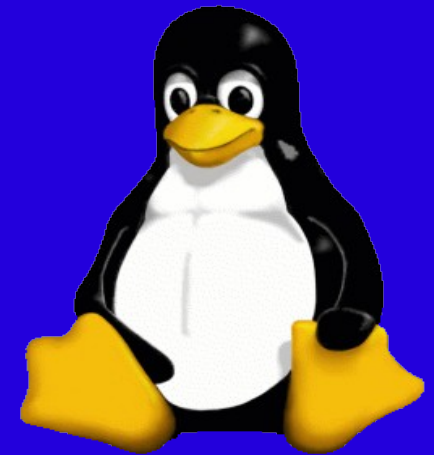


Francesca 2

- 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?

