

## UKHEC Annual Seminar

Progress on the Procurement of HPC(x)

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Project Leader

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## Progress on the Procurement of HPC(x)

Background to HPC(x)

Overview of the SOR

HPC(x) technology benchmarks

Any questions

[www.epsrc.ac.uk/hpc](http://www.epsrc.ac.uk/hpc)

# Large Facilities Strategic Road Map

- Issued by OST in May to contribute to the development of a long term vision of future requirements of the UK Science and Engineering base
- First attempt at a 10-15 year road map of future facility requirements
- Strategic areas covered are:
  - synchrotron radiation
  - neutron beams
  - radioactive particle beams
  - particle physics
  - astronomy
  - oceanographic research vessels
  - computing infrastructure

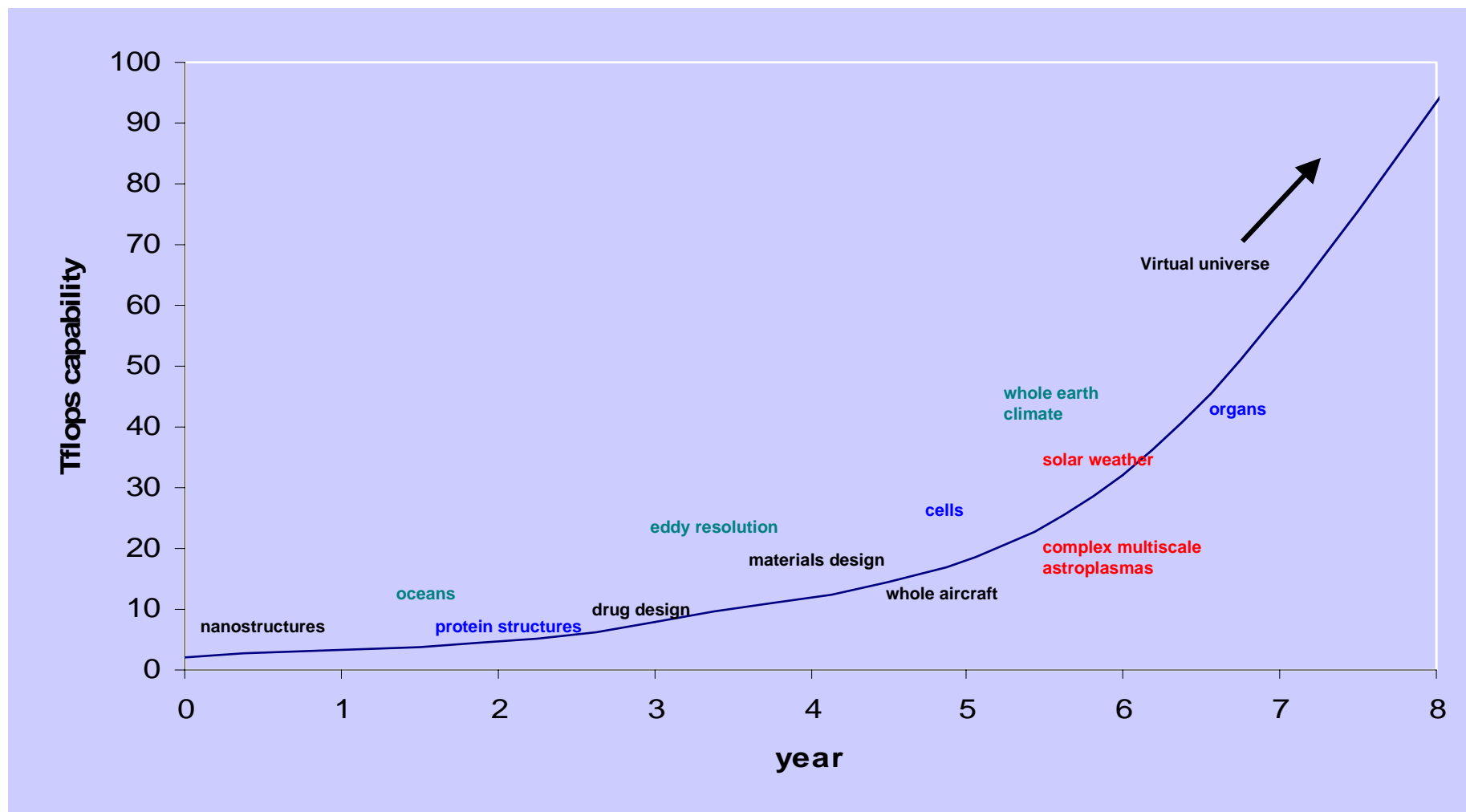
## Computing Infrastructure

- Provision of HEC within the UK has acted as a catalyst for high quality research across a wide range of disciplines
- Roadmap of the USA ASCI programme is to produce machines with 100 Teraflop/s peak performance by 2005
- In Japan, the Earth Simulator project is also being used to drive the technology, with a target of 40 Teraflop/s within the next few years
- Development of Grid computing is intricately linked to the utilisation and exploitation of high-end computing

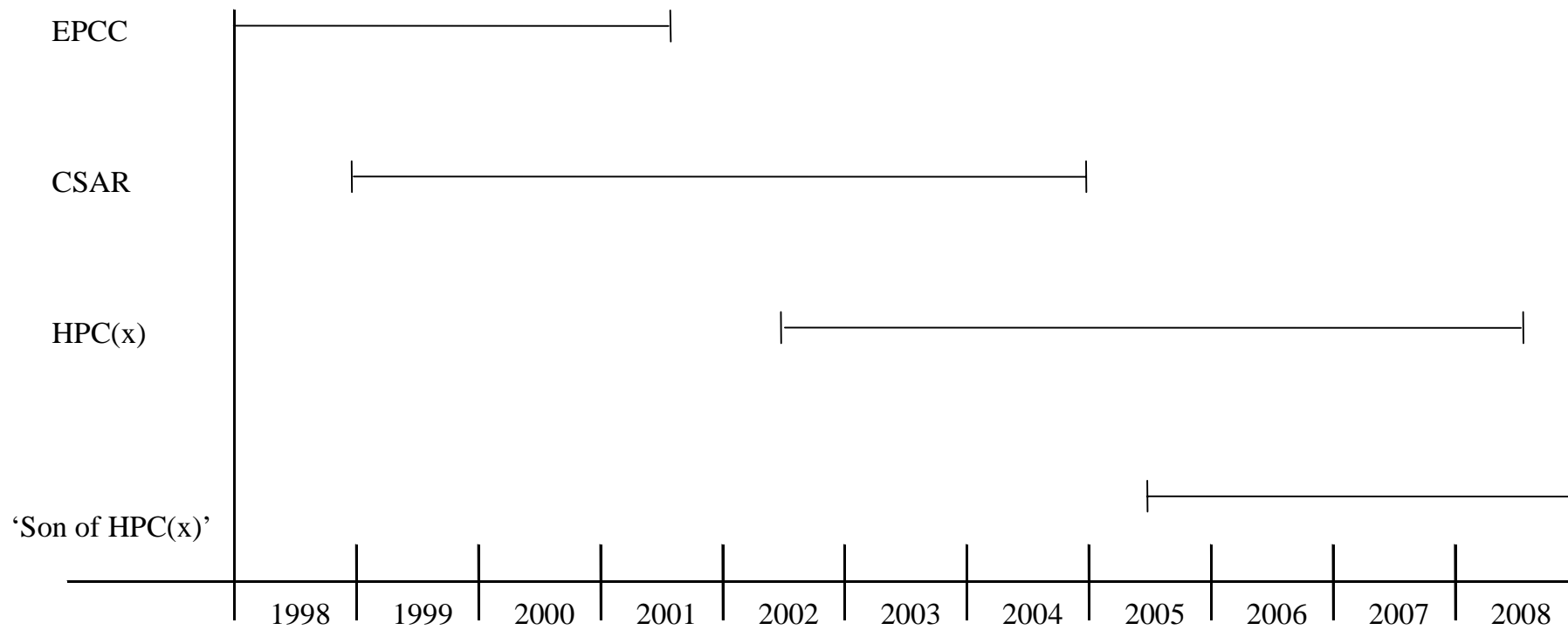
## Rolling Programme of HEC Service Procurements

- Goals for flagship high-end computing facilities are:
  - 5-8 Teraflop/s peak in 2002
  - 20-25 Teraflop/s peak in 2004/05
  - 50-100 Teraflop/s peak in 2007/08
- Facilities linked more closely to particular research communities, eg QCD, computer science, protein folding
- Need for associated support eg, for data management, code development and training for new users

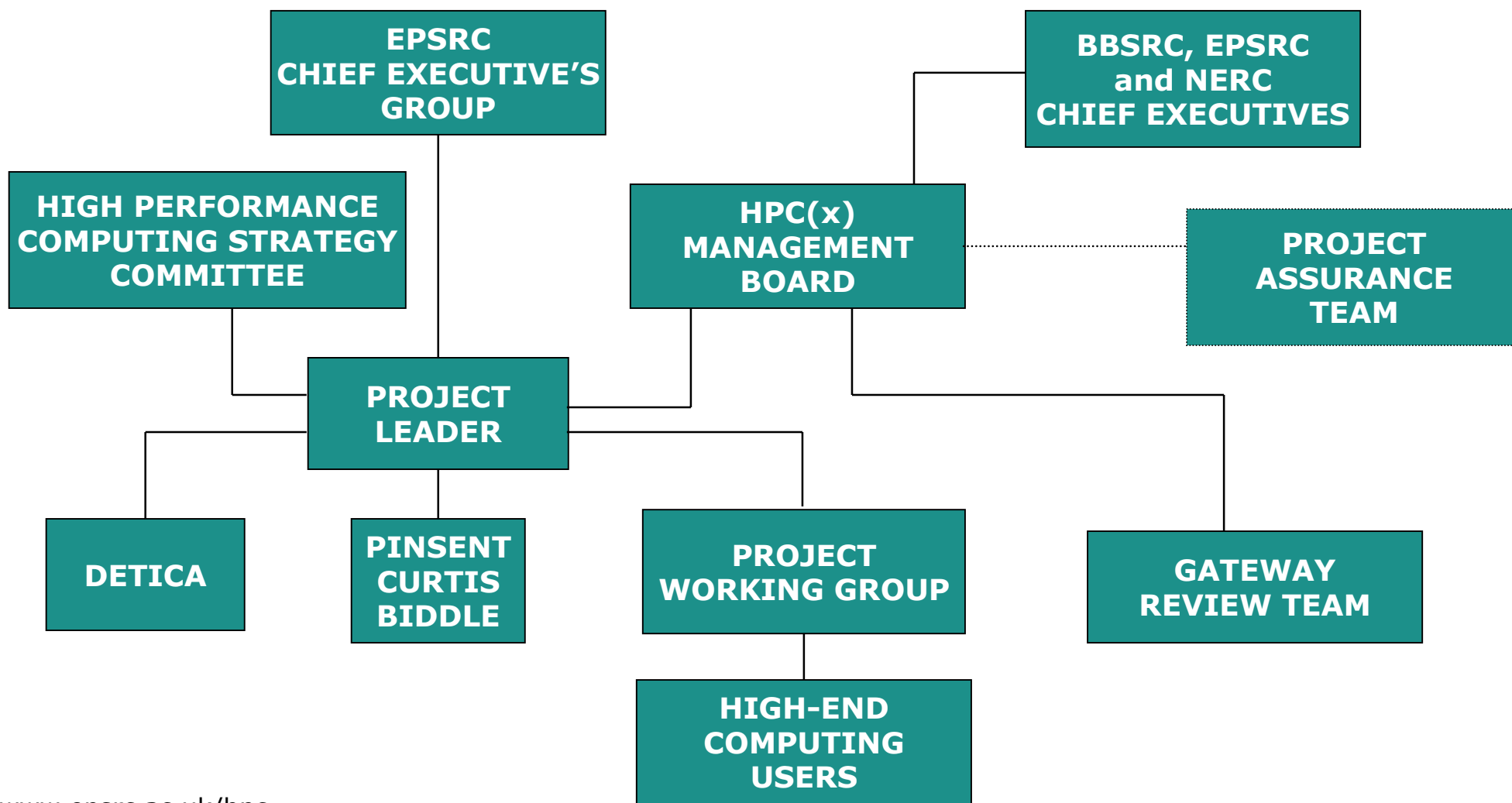
# HEC Scientific Requirements



# HEC National Provision



# HPC(x) Project Structure



## HPC(x) Key Players

Senior Responsible Officer - Dr David Clark, EPSRC

HPC(x) Management Board - Professor John Archer, Heriot-Watt

Professor David Bird, Bath

Dr James Wilson, OST

Professor David Price, UCL

Professor Neil Sandham, Southampton

Dr David Clark, EPSRC

Dr Mark Sansom, Oxford

Professor Richard Catlow, Royal Institution

Representative from the MRC community

Representative from the PPARC community

## HPC(x) Key Players

### Gateway Review Team:

Dr John Stewart	OGC
Professor Ron Perrott	QUB
Professor Ken Taylor	QUB
Dr Fred Hopper	NERC

## HPC(x) Key Players

- Project Working Group
- Mr Hugh Pilcher-Clayton, EPSRC
  - Dr Jon Hunt, EPSRC
  - Mr David Pickett, EPSRC
  - Mr Quentin Vaughan, Detica
  - Dr Carol White, Detica
  - Dr Denis Nicole, Southampton
  - Dr Lois Steenman-Clark, Reading
  - Professor Neil Sandham, Southampton
  - Mr Nick Maltby, Pinsent Curtis Biddle
  - Professor Mike Payne, Cambridge

## Lessons learnt from CSAR

- Overall, a successful application of PFI
- Demand for computing power has exceeded expectations
- Technology Refresh requirement is too low
- Disc storage requirements should be less prescriptive
- Turn-around times need to be guaranteed
- No need for a separate system for pre-post processing
- Value-added services need to be rigorously evaluated

## Lessons learnt from CSAR

- Need an emphasis on capability work
- The Customer Performance Assessment Rating System (CPARS) has been an effective means of ensuring good service quality
- Need to foster the involvement of users in the management structure for the service
- The service must have a clear identity and strong vision
- A robust capacity planning process is necessary
- The service trading pool has been an effective tool
- Need an emphasis on furthering scientific opportunity
- In the light of E-science, there must be collaboration with other service providers

# HPC(x)

## Progress to date

- Decided not to partner with other agencies, end of March
- OJEC advert issued, 2 April
- Responses evaluated at the beginning of June
- Statement of Requirements issued, 29 June
- Responses to the SOR received by 24 August

## HPC(x) Future Timetable

- Issue the Invitation to Negotiate, October
- Negotiations, full assessment, benchmarking phase II, and a decision whether to follow PFI, October to December
- Final assessment and selection, December to February 2002
- Acceptance and establishment of service, June 2002

## Overview of the SOR

- Three separate areas
  - Technology Provision
  - Added Value Services
  - Accommodation Services
  - (plus general requirements)
- Bidders must respond separately for each area
  - shortlisted organisations will have been informed of which component(s) they have been invited to bid against
- Complete responses only will be accepted
- SOR shortlists will be made available to all members on the shortlists

## The general focus

- Capability
  - HPC(X) is to be primarily a capability service
  
- Flexible
  - Impossible to foresee how user requirements will evolve over lifetime of service
  - HPC(X) must recognise this and build in to service
  
- Usability
  - Users must be helped and encouraged to develop codes which make maximum use of service capability

# Technology Provision

- Performance
  - Minimum levels given, but key is responsiveness to the needs of the users
  - All benchmarks must run in a sustained and scaleable way
  
- Installation
  - Full service must be installed within 6 months
  - Phased installation acceptable
  - Full details of upgrade route(s) required
  
- Memory
  - Minimum levels given, but key is responsiveness to the needs of the users

# Technology Provision

## Performance

- Mandatory – a performance of at least 3.0 Tflop/s on the LINPACK benchmark
- Desirable – a performance of at least 2.0 Tflop/s on the ASCI Blue sPPM benchmark
- For system upgrades, a doubling of the mandatory and desirable requirements two years and four years after installation
- Mandatory – the ability to run the suite of user benchmarks

# Technology Provision

## Memory

- Mandatory – 512 GB
- Desirable – 1 TB
- For system upgrades, a doubling of the mandatory and desirable requirements two years and four years after installation

# Technology Provision

- Storage
  - Solution should be flexible and support needs of users
- Backup scenarios envisioned
  - User or system error deletes data
    - restored data no more than 24 hours out of date
  - Catastrophic failure:
    - restored data no more than 7 days out of date
- Reliability, availability and serviceability
  - Note that failure is not just a system failure
- Operating System/ User Environment
  - Rich workstation like environment with C and FORTRAN development environments
  - Rich parallel development environment, key scientific and numerical libraries

# Technology Provision

- GRID technologies
  - Solution should be flexible and support needs of users
  - This needs to be enabled and supported
  
- Network connectivity
  - Bidders to price (separately) cost of connecting to SuperJanet 4
  
- Technology roadmap and leverage off other activities
  - Technology must evolve, but in a sustainable, user-friendly way

## Accommodation Services

- Key to accommodation services is degree of integration with other components
  - technology: physical accommodation, air conditioning, power, network connections, upgrades, support, ...
  - added value: front-line support, reporting, auditing, ...
- Above all: flexibility and responsiveness to user needs

## Added Value Services

- AV services are the key to delivering maximum science through the service:
  - world-leading science
  - support of scientific process
  - training in use of service
  - migration and adaptation of user applications
  
- Key is to work with users
  
- Expected to provide a shop-front for UK science
  
- International collaboration

## HPC(x) technology benchmarks

- Two contractual benchmarks
  - LINPACK, as used in the top 500
  - sPPM, as used for ASCI Blue
  
- Six user benchmarks
  - RAPS
  - CASTEP
  - H2MOL
  - NEWT
  - POLCOMMS
  - AMBER