HPCx
CAPABILITY COMPUTING

Support Services

Overview

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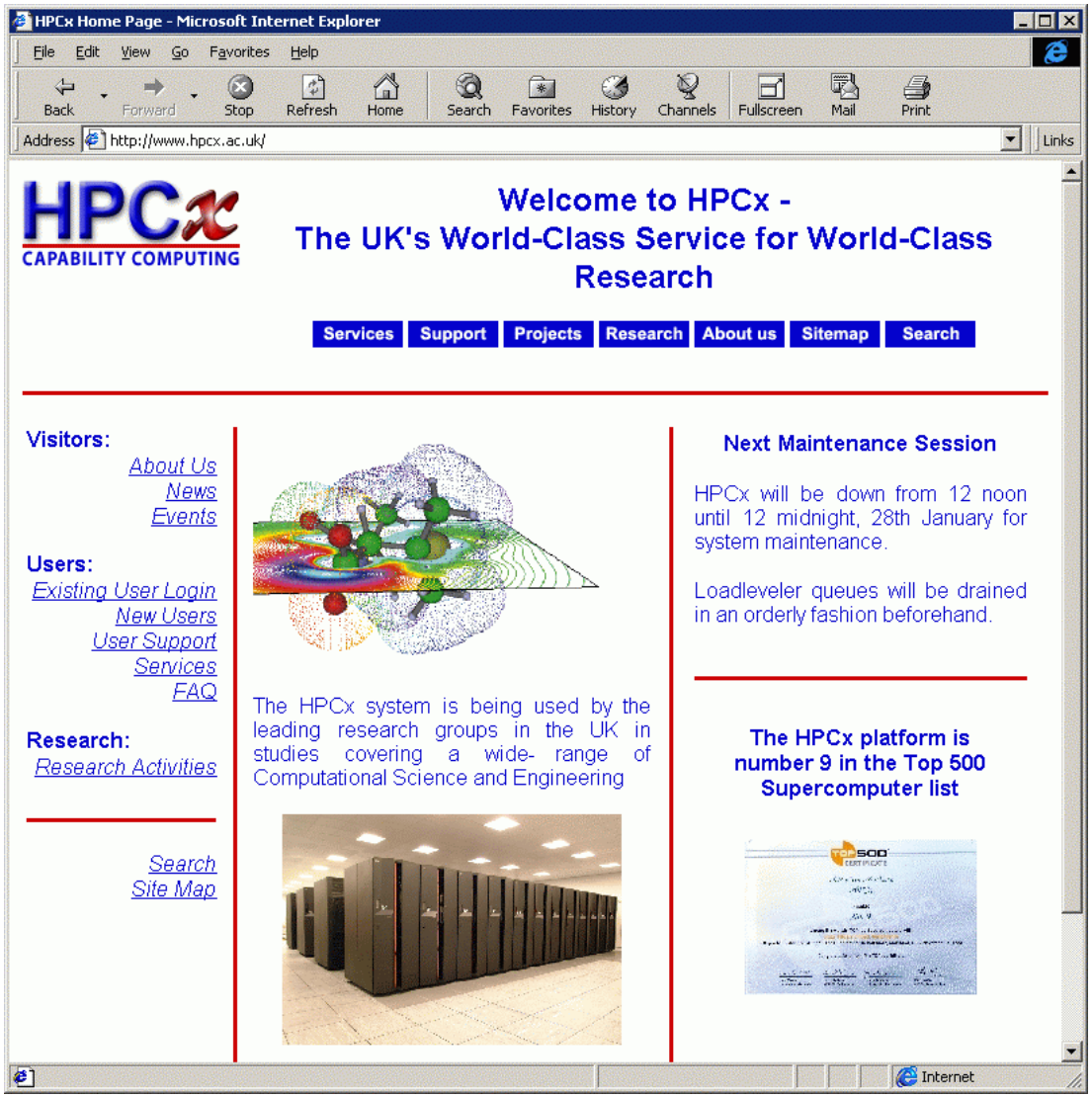
- Web site
- User support information
- Administration service
- Service information
- Conclusions
- References

The Web Site – www.hpcx.ac.uk

HPCx CAPABILITY COMPUTING



The Web Site

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- User support information
  - helpdesk information, user mailings, bulletin board, documentation, training course details, FAQs,..
- Administration service
  - project administration via the admin secure web service
- Service information
  - hardware + software details, current machine status, service policies
- Research information
  - details of research being carried out on the HPCx system
- General information about HPCx
  - news, events, newsletter, HPCx staff

User Support Information

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- HPCx aims to support users via a number of mechanisms:
- Helpdesk
- Functional teams
- Training courses
- Bulletin board

HPCx HelpDesk

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- Provides access to HPCx support team
  - answers questions on using the service
  - mechanism for providing comments and criticisms
- Queries can be submitted via:
  - email: **support@hpcx.ac.uk**
  - web submission form:
    http://www.hpcx.ac.uk/support/helpdesk/query.html
  - by phone: 0131 650 5029
  - by fax: 0131 650 6710
  - by post

HPCx HelpDesk

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- HelpDesk software banks and tracks queries
- Queries
  - (email and web based queries) receive an automatic response within minutes
    - query has arrived at the helpdesk, query number assigned
  - helpdesk operator assigns query to an “expert”
    - expert receives copy of the query
    - expert may contact you directly to discuss the query
    - expert sends you an answer
  - helpdesk operator finishes the query
    - you receive an e-mail telling you this has happened
    - records of queries are retained indefinitely

Service Level Agreement (SLA)

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- The SLA states that queries must be answered within a certain time:
  - 97% of Admin queries within 2 days
  - 75% of all queries within 1 day
  - 97% of all queries within 3 days
- Some queries may be marked as 'in-depth' - no time limit. For example:
  - queries requiring more than 1 person-day of work
  - queries requiring more input from the user
  - queries requiring referral to a 3rd party

Functional Teams

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- Dual centre teams to address key targets
- Terascaling applications
  - collaborating with users to develop capability applications to exploit HPCx facilities
  - developing highly scalable numerical algorithms
- Software engineering
  - ensuring portable, high-quality code development
  - interfacing with emerging computational Grid

Functional Teams

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- New applications outreach
  - spreading the use of HPC to new applications and other Research Councils, eg, Life Sciences
  - supported by IBM Life Sciences, Accelrys, …
- Applications support
  - ensuring service meets the users' needs
  - co-ordinating support activities, eg, helpdesk and training, and other teams
- Operations and systems
  - delivering a flexible capability computing service
  - ensuring smooth transitions between phases

Key HPCx staff

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- Functional teams and queries primarily involve the following staff
  - Alan Simpson (project director)
  - Richard Blake, Stephen Booth, Mike Brown, Martyn Guest, David Henty (team leaders)
  - Mike Ashworth, Mark Bull, Ian Bush, John Fisher, Joachim Hein, Martin Plummer, Gavin Pringle, Fiona Reid, Lorna Smith, Andrew Sunderland, Alan Gray, Huub vanDam, Kenton D'Mellow, Paul Sherwood, Jon Hill,…
- Experienced in HPC and e-Science. . .
  - . . . and in a broad range of application fields
- See:
  - **http://www.hpcx.ac.uk/about/staff/**

Training

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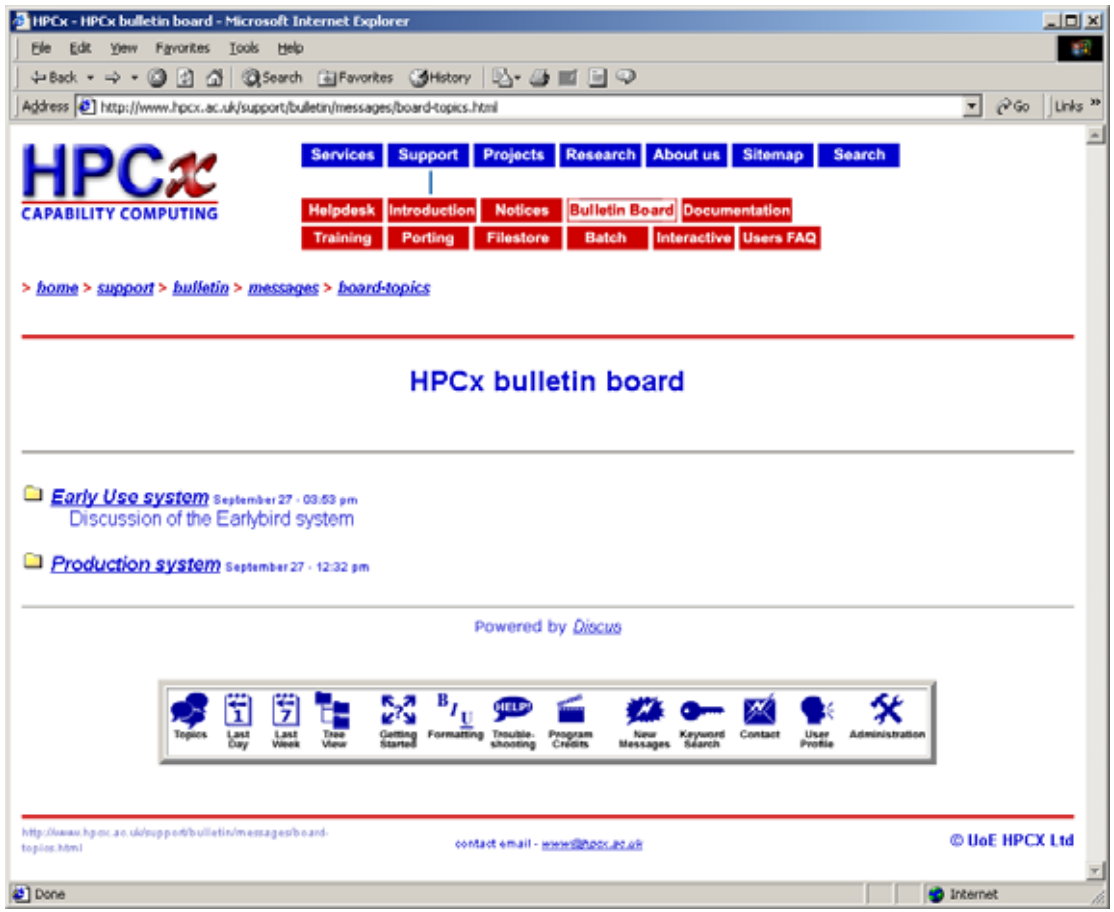
- Majority of existing courses available to HPCx users
  - MPI, OpenMP, languages, algorithms, …
- New training courses
  - Using the HPCx service
  - Performance Optimisation
    - compiler switches, cache management, loop structure, …
  - Terascaling
    - optimal use of MPI, LAPI, shared-memory tricks, ..
- Application and discipline specific workshops
- See:
  - **http://www.hpcx.ac.uk/support/training/**

Bulletin Board

- Allows exchange of information between HPCx and our users and PIs



Administration Service

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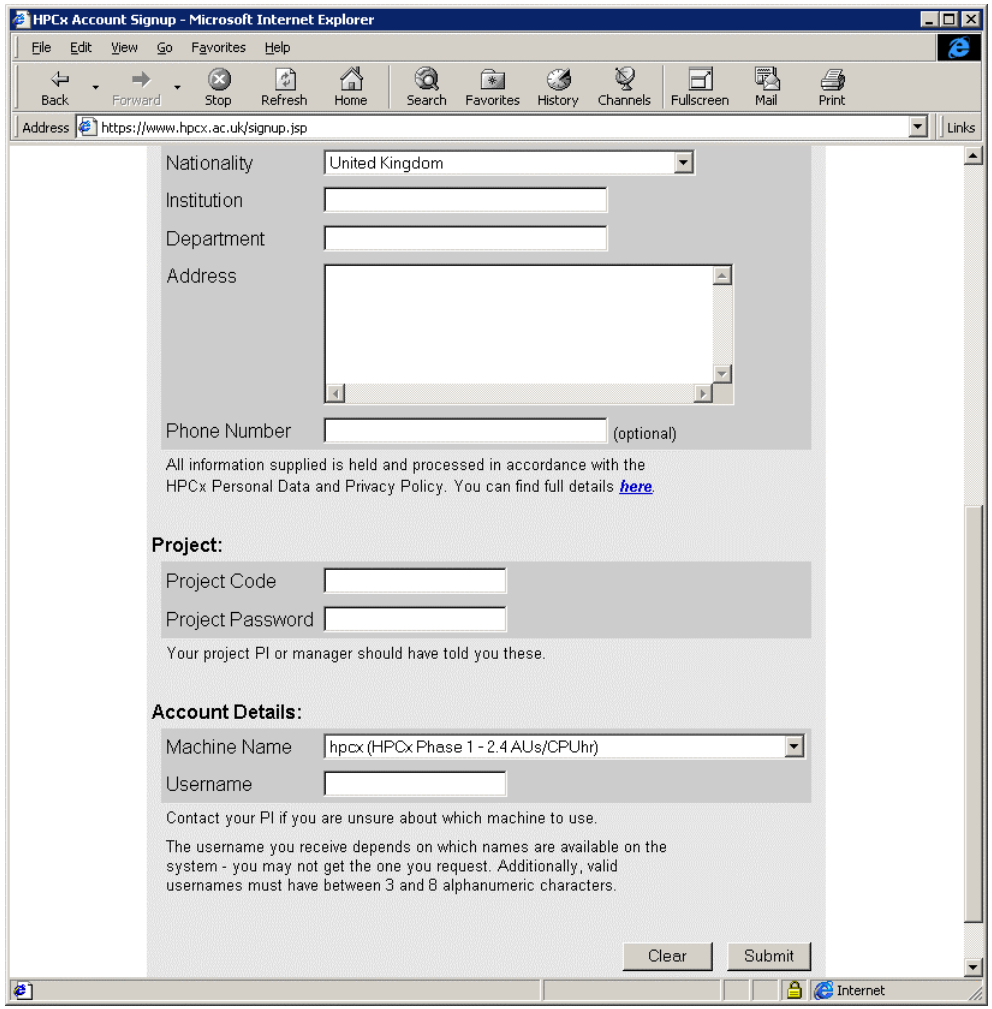
- A secure web-based system that allows
  - New users to access the service
    - Creating a new account on the administration service
      - identified by unique email address
    - Requesting a user account on a service machine
      - join a project with a new login name
    - Monitoring resource usage
  - PI/Project Managers to manage their resources
    - New-user authorisation, PM pro/demotion
    - Sharing out CPU time and disc space
    - Monitoring and producing reports on resource usage
- Secure server's address
  - **https://www.hpcx.ac.uk/**
  - For information see:
  - **http://www.hpcx.ac.uk/projects/ or http://www.hpcx.ac.uk/projects/FAQ/**

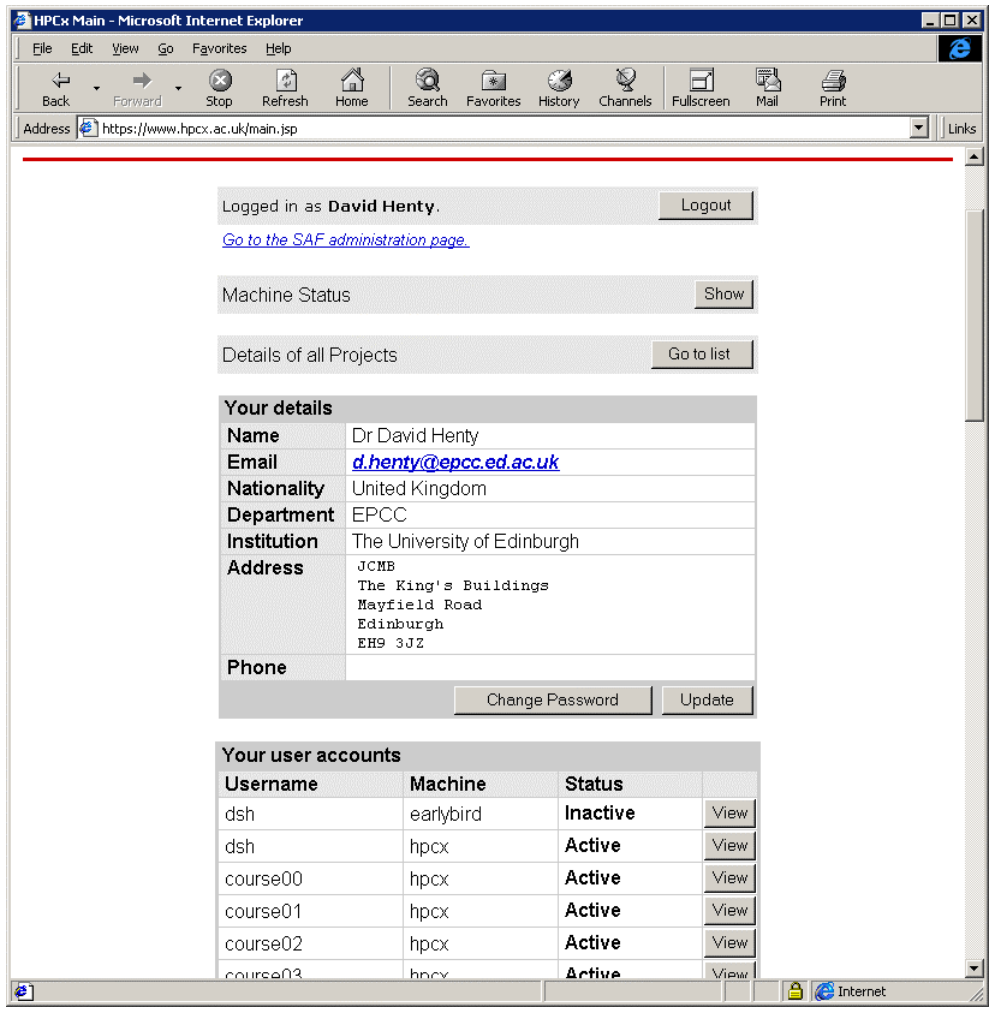
New User Registration 1/3

- User opens Admin Service account
  - requests an account on a service machine
  - requires project name & password
- Admin Service
  - emails admin service password to user
  - emails project manager/PI for confirmation



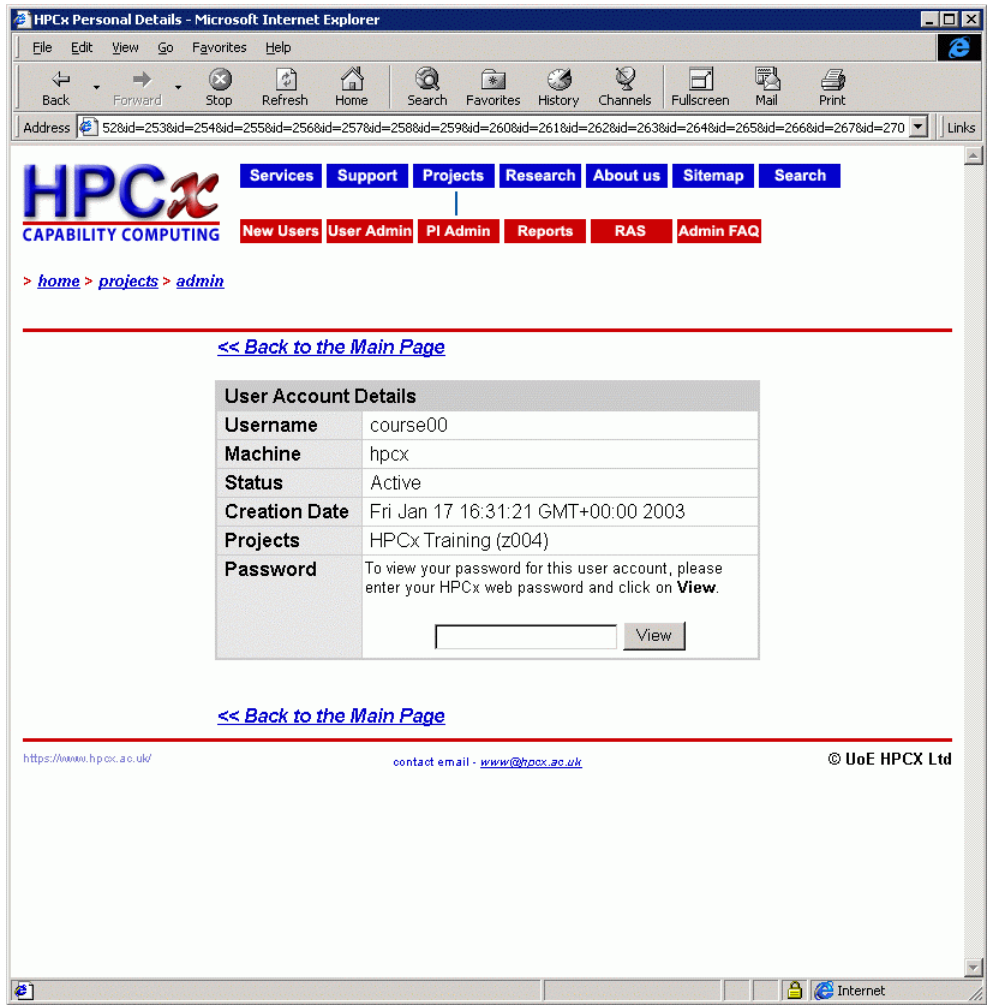
New User Registration 2/3

- The PI/Project Manager
  - logs on to the Admin Service
  - confirms the creation of the user account
- When confirmed
  - Admin Service emails System support staff
  - they create an account



New User Registration 3/3

- After creating the account
  - system support staff tells the Admin Server that the account has been created & what the password is
- The Admin server emails user
  - informing them that the account is ready
- User can then use the Admin server to look up the password



PIs & Project Management

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- Confirming new users
- Creating sub-projects, to split resources between different sets of users
- Nominating (sub-) project managers
  - Who can do everything that PIs can
- Storing resources in a "reserve budget"
  - For use later in the funding period
- Adding/changing resources for different (sub-) projects
  - Both CPU-time and disk space

Service Information

- See:
  - **http://www.hpcx.ac.uk/services/**
- Service policies
  - capability incentives
  - charging model
  - also
    - contingency and revision plan, data backup, personal data and privacy policy, information security policy
- HPCx and the Grid
- Packages
- Also hardware and software details, current machine status, …

Service Policies – Capability Incentives

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- EPSRC's objectives for the procurement were to
  - aim "to deliver the optimum service resulting in world-leading science"
  - address "the problems involved in scaling existing codes to the capability levels required"
- Capability Computing
  - jobs which use a significant fraction of the resource
  - eg, at least 512 CPUs
- The challenges we face are to
  - support change from capacity to capability
  - develop more scalable codes

Capability Incentives

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- Codes reviewed by science support staff
  - award a 'seal of approval' at one of three different levels
  - discount provided for each seal of approval level

Level	No of Processors	Discount
Bronze	256	5%
Silver	512	15%
Gold	1024	30%

- Satisfactory scaling an important criterion
- Any disagreements will be passed to the EPSRC
- See:
  - http://www.hpcx.ac.uk/services/policies/capability.html

Charging Model

- Charges will be calculated on the amount of CPU time used
- Charges will be in terms of a standard "Allocation Unit" of CPU time
  - equivalent to 1 gigaflop processor running for 1 hour
  - constant throughout the service
  - Currently 1 AU is roughly 0.21 CPU hours
- See:

  http://www.hpcx.ac.uk/services/policies/charging_model.html

Grid Software

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- Software engineering team
  - help users to Grid-enable codes
  - strong links with e-Science centres

- HPCx on the Grid
  - Globus 2.4.3 is running on HPCx

Packages

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- HPCx supports a number of software packages, available pre-compiled
  - AMBER
  - CFX
  - DL_POLY
  - NAMD
  - GAMESS-UK
  - VASP
  - SIESTA
  - LAMMPS
  - and many more…
- Information on codes for specific application areas at
  - http://www.hpcx.ac.uk/research/
- Licenses required for some codes
- Contact the Helpdesk for further information

Conclusions

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- HPCx aims to provide support for users via a number of mechanisms:
  - web site
  - helpdesk
  - functional teams
  - training and documentation
  - bulletin boards
  - administration service
- Have summarised:
  - service level policies
  - Grid status
  - application packages

Overall Conclusions

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- This course has:

- introduced the HPCx architecture
- described the steps involved in compilation
- explained how to submit batch jobs
- highlighted the different tools and libraries available on the system
- summarised the different user support mechanisms available

References

- See the HPCx web site:

  http://www.hpcx.ac.uk