

Computing @SERC
Resources, Services and Policies



R. Krishna Murthy

SERC - An Introduction

- A state-of-the-art Computing facility
- Caters to the computing needs of education and research at the institute
- Comprehensive range of systems to cater to a wide spectrum of computing requirements.
- Excellent infrastructure supports uninterrupted computing - anywhere, all times.

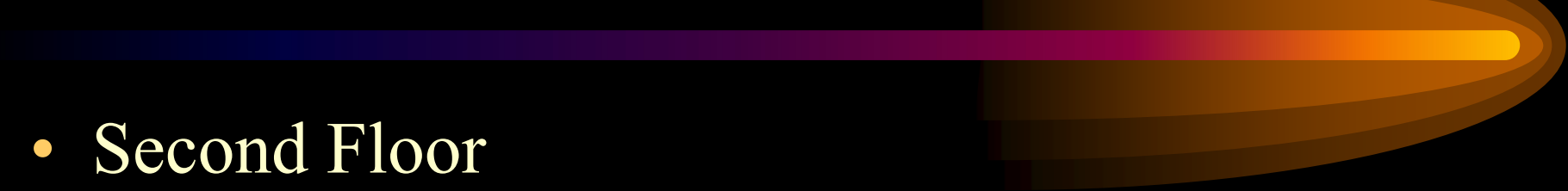
SERC - Facilities

- Computing -
 - Powerful hardware with adequate resources
 - Excellent Systems and Application Software, tools and libraries
- Printing, Plotting and Scanning services
- Help-Desk - User Consultancy and Support
- Library - Books, Manuals, Software,

Distribution of Systems

- SERC has 5 floors - Basement, Ground, First, Second and Third
- Basement - Power and Airconditioning
- Ground - Compute & File servers, Supercomputing Cluster
- First floor - Common facilities for Course and Research - Windows, Unix / Linux workstations

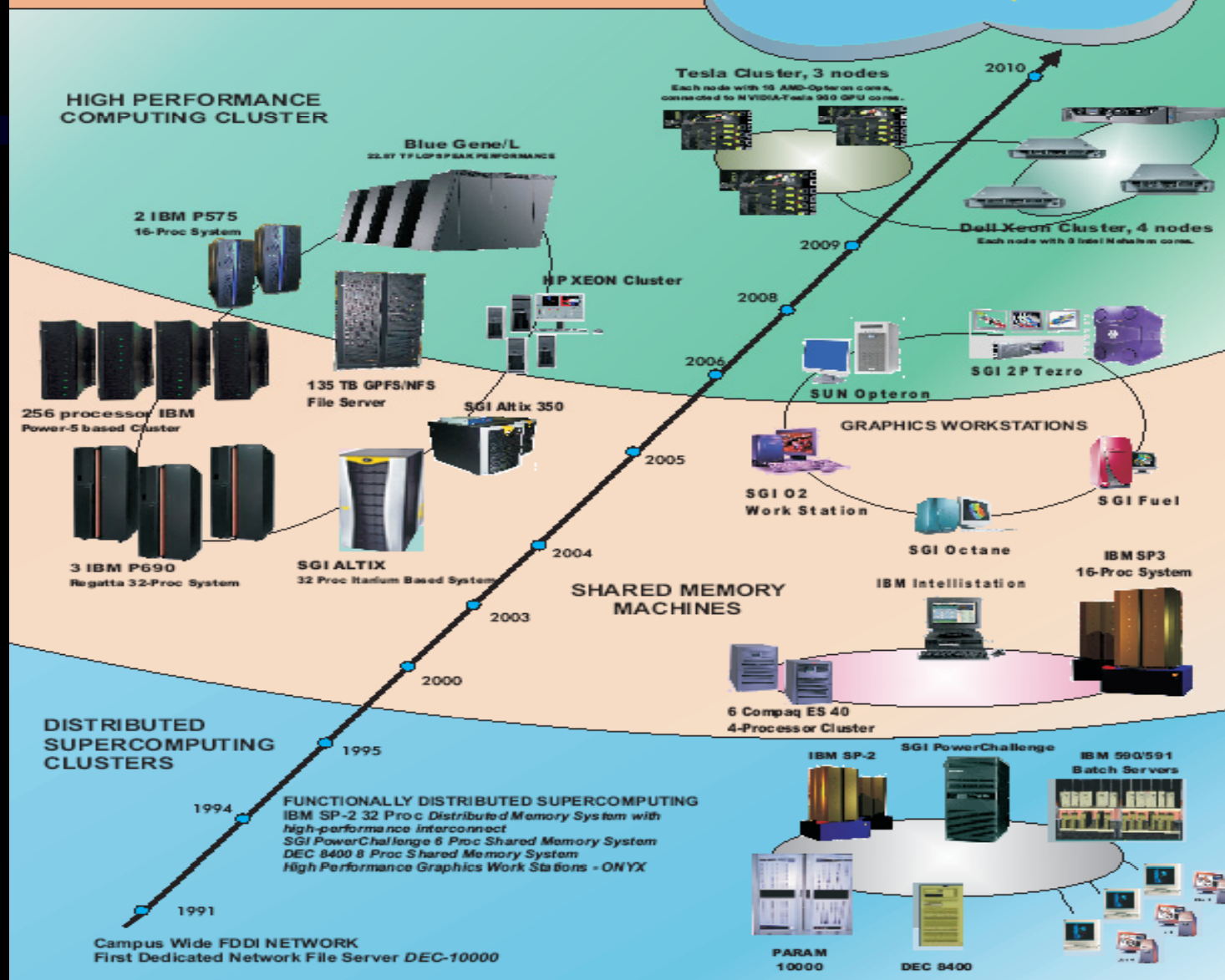
Distribution of Systems - contd.

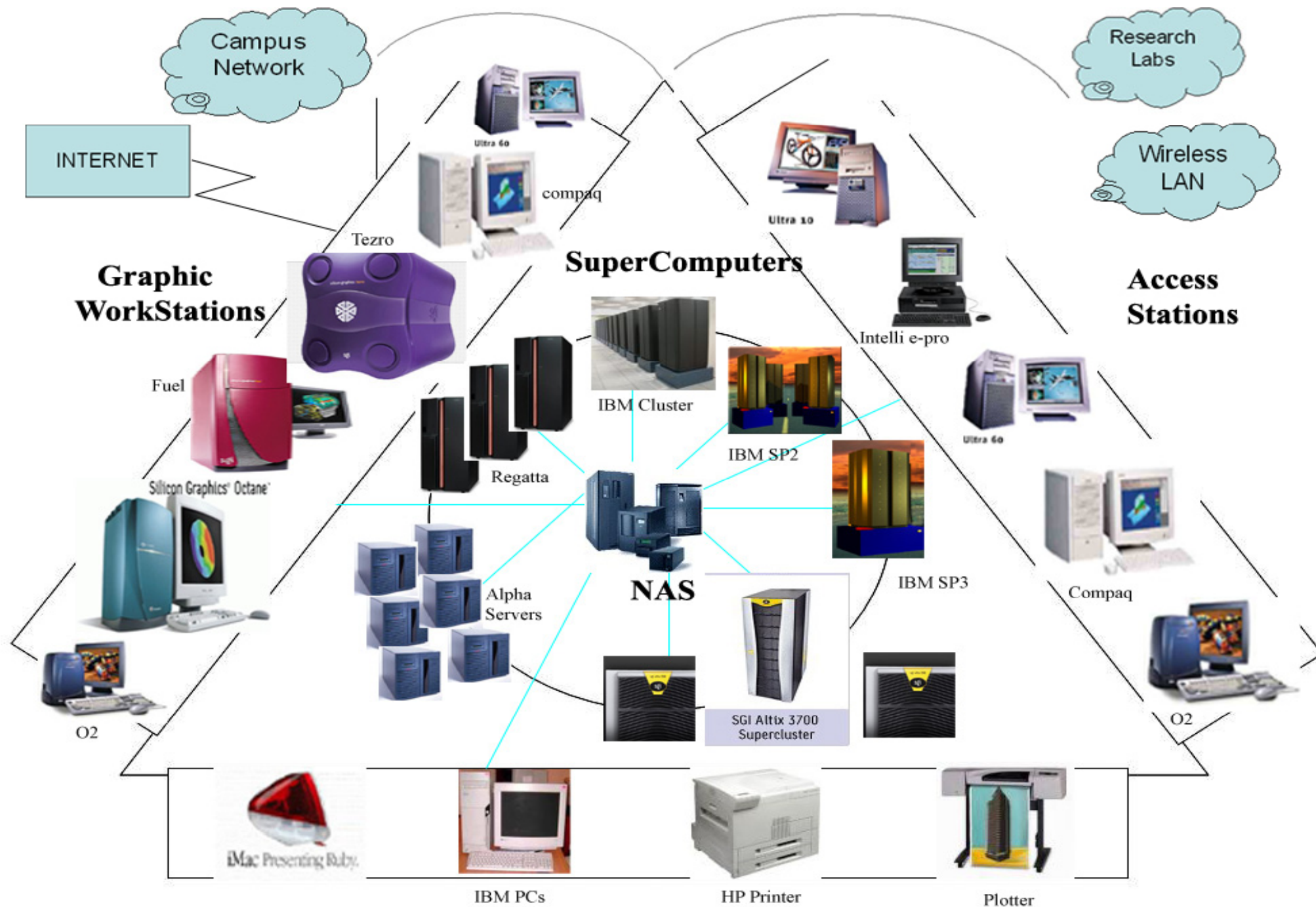


- Second Floor
 - Primarily Unix/Linux access stations. Originally used by research students
- Both the floors have similar facilities
- Third Floor - Labs

Evolution of Computing@SERC

- State-of-the-Art Computing Systems with Sophisticated Software Packages
- Listed in the Top500 computing centres of the world.
- Symbiosis of computing, storage, network and graphics & visualization.
- Dedicated power and air-conditioning infrastructure for 24x7/365 operation





Systems at SERC



- *ACCESS STATIONS*
 - Program development, executing applications requiring less resources
 - Browsing, visualization
 - Access the more powerful systems like HPC clusters for submitting jobs for batch processing
- Basic access – provided for all users



FILE SERVERS

130 TB SAN storage

**Users Home storage, Scratch Area, System and
Application software**

- HIGH PERFORMANCE SERVERS

Primarily used for resource intensive Batch mode computing

- * *SHARED MEMORY MULTI PROCESSOR*

- IBM P-series 690 Regatta (32proc.,256 GB)
 - SGI ALTIX 3700 (32proc.,256GB)
 - SGI Altix 350 (16 proc.,16GB – 64GB)

- *DISTRIBUTED MEMORY*

IBM P720 64 node , 256 processor Cluster

4 CPUs / node - 1.65 GHz

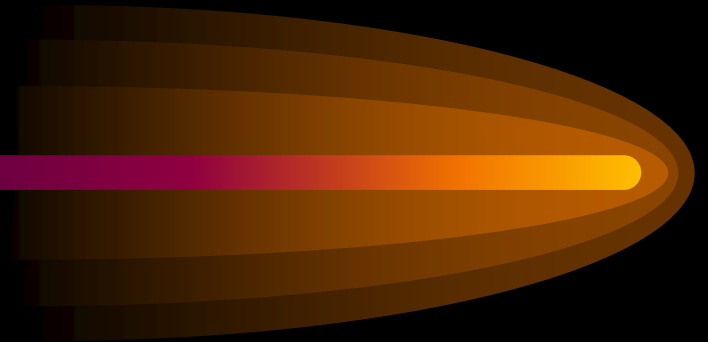
- **HIGH PERF. GRAPHICS STATIONS:**

- ☐ **SGI TEZROs and FUELS**
- ☐ **SGI OCTANE**
- ☐ **SGI ONYX WORKSTATIONS**

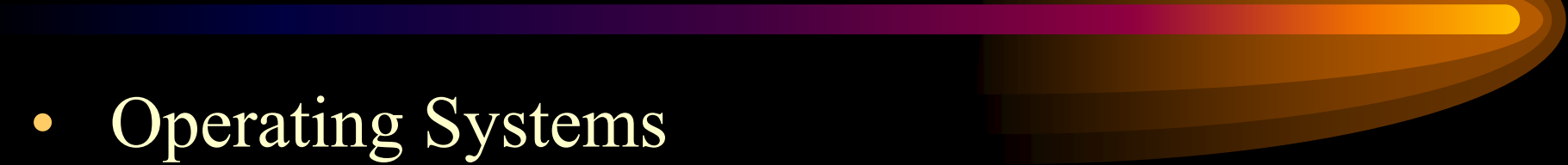
- **Networking within SERC**

- **Gigabit network to the desktop**
- **Wireless network access**

- Campus Network



Software at SERC



- Operating Systems
 - Unix / Linux
 - Windows
 - Aix

- Numerical packages and Libraries

- MATLAB
- MATHEMATICA
- MAPLE
- ESSL

- Programming Tools

- Compilers : C, C++, Fortran, java., GNU gcc
- Debuggers : dbx, xldb, GNU's gdb

Contd...

- Special-Purpose packages

- FEM SOFTWARE

- Quantum chemistry packages

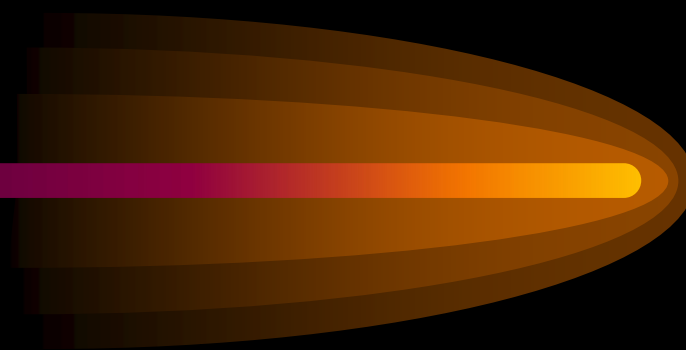
- Gaussian 03 , Gaussian 09

- Molecular Simulation software

- Insight II (Biosim etc.)

- Schrodinger software suite – drug discovery

- Molecular Operating Environment – tool for
Chemical Computing Software development and
deployment



Printing Services

→ Printing is a chargeable facility

- Laser Printers - HP Laser Jet 8100 DN
- Color Printers – HP Design jet 500PS(A0), HP KPro 850, Xerox Phasor 6200 N
- Scanners – Umax scanner(upto 9600 dpi) , A4, A3 size, High resolution, including negatives and slides .

User Consultancy



- Help Desk - 444
- Help in using the system
- Problem resolution
- Support on the floor
- Program development, optimization, porting
- Backup services

Documentation



- On-Line Documentation
 - Man Pages
- Hard Copy Documentation
 - Limited - Available in SERC library
- CD-ROMs

Modes of Computing



- Interactive
 - user interacts with his job directly
 - eg. Program Development
 - Uses workstation or logs on to server
- Batch
 - User submits a command file for queued processing
 - No direct interaction. Eg. resource intensive jobs
 - uses the batch facility - Loadleveler, LSF, PBS-pro

Using the Facility

- Who can use the facility ?
- How to gain access? Obtain an Account
 - Choose the right form, complete and submit to SERC
- When you are allotted an account you get
 - User-Id, Password,
 - Resources like disk space and access to a subset of systems at SERC

Computing Resources

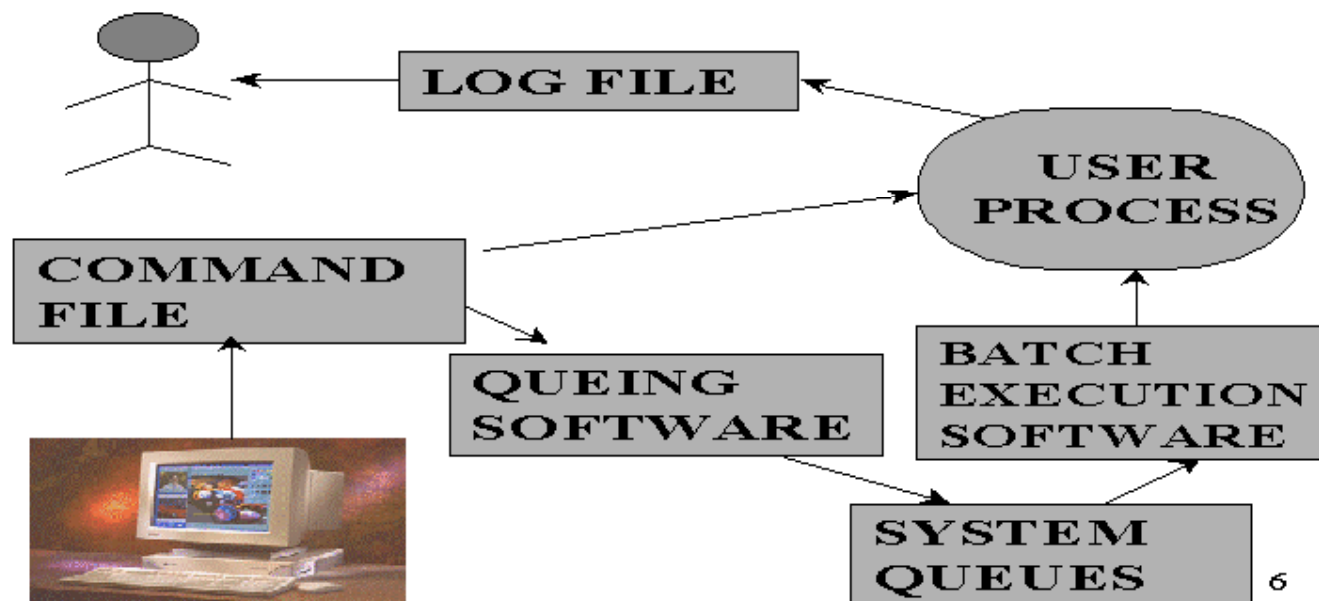


- CPU - Hours, Minutes, Seconds
- Memory - KB, MB
- Disk Space - Blocks, MB, GB
- No. Of Files
- Swap Space - MB, GB
- Connect Time - Hours, Minutes, Seconds

Interactive Mode



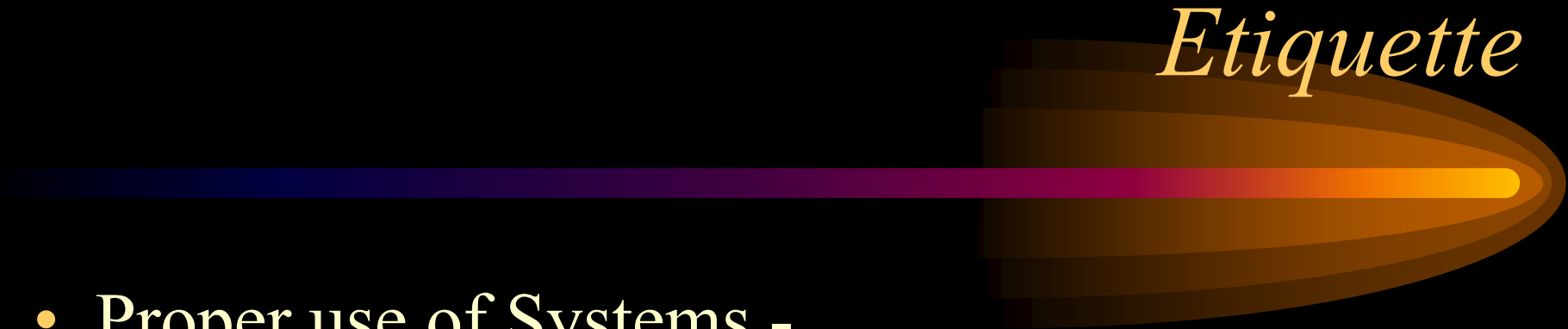
BATCH MODE



Policies

- Policies are introduced ONLY to facilitate convenient ,smooth and effective usage.
- Policies change to reflect changing requirements.
- User's inputs help us in formulating effective policies
- Policy and other info. Communicated through notices, Message-of-the Day(motd), e-mail broadcast

Usage Policies and Computing Etiquette



- Proper use of Systems -
 - Handling systems with care
 - Escalating problems to Help desk and operating staff
 - Do Not rearrange systems
 - Do Not switch off/ reset or attempt to connect/disconnect components.
 - Crowding space around systems with books , water bottles etc.

Love Thy Neighbour

- Be sensitive to the needs of fellow users
 - Resources are finite - use them , *don't lock them*
 - Playing audio files disturbs users
 - Computing and eating do not mix -eatables attract rodents, insects - they don't use computers for solving problems they love creating problems for computers
 - Systems are expensive, treat them with respect
 - Don't use them as book rest, foot rest etc.

Resource Usage



- Resources are finite , use them effectively
- Do not run Background jobs
- Release disk space in Common areas like /tmp etc. promptly
- Resource intensive non-interactive jobs on systems meant for interactive use cause response deterioration

Resource Allocation

- Resources Allocated, based on computing needs on systems which are best suited for satisfying these requirements.
- Different groups have different needs
- Default Resource Allocation
- Additional Allocation
 - 1. Short term (a few days) 2. Long term
 - Faster Response to 1.

Resource Utilization

Very often increased resource requirements can be avoided by

- using compiler optimization switches
- reorganizing code ,data
- using better algorithms

Disk space requirements can be reduced

- compressing files

No. of files restriction can be avoided by using tar utility

Security



Physical Security

- Signing in/off at the Security Desk
- Producing the identity card on request by staff
- Leaving your bags before moving on to the computing floor.
 - All these are required to facilitate maintenance of security

Security - contd.

- You are responsible for all usage arising from your account - even its misuse by others.
- Anyone who can provide your userid/password combination can use your account
- Choose good passwords and frequently change them . Use Password checker
- You login to access a system for use. After use you *have to logout*.

Security - contd.

- Not logging off and leaving unattended interactive sessions are sure ways of inviting avoidable disasters
- Protect your information and backup important info.
- Obtain your customization files from reliable sources
- Ensure that the software you download/borrow are safe and are from reliable sources

User Participation

- *Users play an important role in making the centre a useful and effective facility*
- *Please provide valuable feedback*
 - *on your requirements - h/w ,software*
 - *on the health of systems to enable quick remedial action*
 - *on usage policies*
 - *on things which help you use the system and those that prevent effective use*



*Participate - Help us meet your
Computing Requirements effectively*

Thank You