# ICT AS A TOOL FOR COLLABORATION IN CHEMISTRY

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### Traditional ways of teaching and collaborating in chemistry

- Book and paper disadvantages: a lot of imagination is required for simulations etc.
- Attending seminars (like this one): Can be very expensive unless sponsored.
- Sending documents by Postal mail in Africa –and particularly Kenya, your mail may never arrive. Or it has been tampered with as someone somewhere tries to see whether there are valuables concealed.

 Around the eighties, the Personal Computer became readily available. It was easy to process information on your computer, then carry information in a floppy disk (double density), then high density, CD ROM, DVD, now flash disk.

- The world wide web in the 1990's accelerated the sharing of information between people.
- Email revolutionized the transfer of information between computers,
- Introduction of file attachments made it possible for any document (file) to be attached to an email, and be delivered to the intended recipient at minimum cost.

- However, malicious programs have also been sent via world wide web
- Your documents may contain the data you want, plus harmful additions (viruses) which would alter the data and the computer.
- You may also get unwanted emails (junk) generated by computer scripts with fake addresses.

- Web hosting: Used to be done on expensive servers
- Now it is possible to transform your laptop or PC into a webserver without computing knowledge.

#### **ICT**

- Information and Communications Technology (ICT) is an umbrella term that includes all technologies for the manipulation and communication of information.
- The term is sometimes used in preference to Information Technology (IT), particularly in two communities:
  - Education
  - Government (e.g. in Kenya <u>www.ict.go.ke</u>)

ICT in fact encompasses any medium to record information:

- magnetic disk/tape,
- optical disks (CD/DVD),
- flash memory etc
- technology for broadcasting information radio, television

#### ICT

- Technology for communicating through voice and sound or images - microphone, camera, loudspeaker, telephone to cellular phones.
- It includes the wide variety of computing hardware (PCs, servers, mainframes, networked storage);
- The rapidly developing personal hardware market comprising mobile phones, personal devices such as the BlackBerry; MP3 players such as Apple's iPod.

# Theory: Computers and programming languages

- Computer hardware: This is the physical part of a computer
- Computer programs (software programs): These are instructions for computer.
- The instructions are processed by a central processing unit within the computer hardware.
- Computer programs may be categorized into:
  - System software
  - Application software.

- Many computer programs may run simultaneously on a single computer (multitasking).
- System software (operating system) manages and coordinates the activities and the sharing of the resources of the computer.

#### Common operating systems

- Microsoft Windows,
- Mac OS X,
- Linux
- Solaris.

#### History of internet

- The Internet and the World Wide Web are not one and the same.
- The Internet is a collection of interconnected computer networks, linked by conducting wires, fiber-optic cables and wireless (radio) connections.

 The World Wide Web is a collection of interconnected documents and other resources, linked by hyperlinks.

 The World Wide Web is one of the services accessible via the Internet, along with various others including e-mail and file sharing.

#### Distinctions between the items on the internet:

- Web documents: (http://www.webhost.tld (or territory code)
- File sharing: (ftp://
- Email: yourname@webhost.tld (or territory code)

### Brief history of Internet

- In 1965 a TX-2 computer in Massachusetts to the Q-32 in California with a low speed dial-up telephone line.
- In October 1972 a large, very successful demonstration of the Advanced Research Projects Agency Network (ARPANET, which started in 1969, as a set of four host computers were connected together) at the International Computer Communication Conference (ICCC).

### Brief history of Internet

- This was the first public demonstration of this new network technology to the public.
- It was also in 1972 that the initial "hot" application, electronic mail, was introduced.

### Brief history of www

- In 1980, Englishman Tim Berners-Lee, at CERN, Switzerland built, a personal database of people and software models known as ENQUIRE, as a way to play with hypertext.
- It took 10 years (Christmas 1990), for Berners-Lee to build all the tools necessary for a working Web: the first Web browser, WorldWideWeb (which was also a Web editor), the first Web server (info.cern.ch), and the first Web pages that described the project itself.

### Brief history of www

- The turning point for the World Wide Web was the introduction of the Mosaic web browser in 1993.
- By 1996 it became obvious to most publicly traded companies that a public Web presence was no longer optional.
- By around 2000 emergence of don-com companies which later went bust accelerated the growth of www.
   Currently, search engines like Google, and e-commerce applications have once again made www a commercially viable information superhighway.

#### Local area network

- A local-area network is a computer network covering a small geographic area, like a home, office, or group of buildings e.g. a university.
- Defining characteristics of LANs, in contrast to wide-area networks (WANs), include:
- much higher data-transfer rates,
- smaller geographic range,
- lack of a need for leased telecommunication lines.

#### Wireless LAN

- This is the linking of two or more computers or devices without using wires.
- Benefits
  - Convenience
  - Mobility
  - Deployment
  - Expandability
  - Cost

#### **Disadvantages**

- Security: Wireless LAN transceivers are designed to serve computers throughout a structure with uninterrupted service using radio frequencies.
- Range: The typical range of a standard equipment is on the order of tens of metres. While sufficient for a typical home, it will be insufficient in a larger structure. To obtain additional range, repeaters or additional access points will have to be purchased.
- Reliability: Like any radio frequency transmission, wireless networking signals are subject to a wide variety of interference that are beyond the control of the network administrator.
- Speed: The speed on most wireless networks (typically 1-108 Mbit/s) is reasonably slow compared to the slowest common wired networks (100 Mbit/s up to several Gbit/s).

### Wireless security...

- Wireless networks are little more secure than wired ones; in many offices intruders can easily visit and hook up their own computer to the wired network without problems, gaining access to the network, and it's also often possible for remote intruders to gain access to the network through backdoors.
- One general solution may be end-to-end encryption, with independent authentication on all resources that shouldn't be available to the public.

### Different computing languages used to manage content on the web

- HyperText Markup Language (HTML)
- It is the computer language used to create hypertext documents, allowing connections from one document or Internet page to numerous others. HTML is the primary language used to create pages on the World Wide Web.
- It is a cross-platform text-formatting system for creating web pages, including copy, images, sounds, frames, animation and more.
- It is a set of tags and rules used in developing hypertext documents to be presented on the World Wide Web.
- Internet browsers read HTML to know what they should display.

### Example of HTML

```
<html>
<head>
<title>Hello Ladies and Gentlemen</title>
</head>
<body>
<center>
<h1>
Hello Ladies and Gentlemen!
</h1>
</center>
</body>
</html>
```

#### **JavaScript**

- JavaScript is a scripting language (list of commands within a program or an application that directs the program to perform specific tasks in a specific order) developed by Netscape.
- It can make web pages more animated and dynamic in terms of graphics and navigation.
- JavaScript code is inserted directly into the HTML page. It is also a programming language for use in web pages that allows the use of dynamic content.
- It can be used for example to respond to user actions such as button clicks or to run processes locally or validate data.

#### PHP

- PHP (Hypertext Preprocessor) -an open source programming language that allows web developers to create dynamic content that interacts with databases.
- PHP is basically used for developing web based software applications.
- It is a scripting language that is executed on the web server (requires a PHP enabled web host).
- PHP commands are embedded within the HTML of a Web page and is useful in the arena of dynamically generated pages.
- PHP scripting can add numerous interactive elements to a website.

#### **MySQL**

- A database is defined as an organized collection of data.
- MySQL is a Database Management System (DBMS) for both Linux and Windows.
- It is Database management software commonly used to store information for use on web sites.
- MySQL is one of the most popular databases for use on the Internet.
- Server side programming languages such as PHP are typically used in conjunction with MySQL to deliver database information over the web.

#### **WEBSERVER**

 Webserver is a software that delivers Web pages and other documents to browsers using the HTTP protocol

#### Apache

- It is the most popular HTTP web server used to serve both static and dynamic web pages on the internet.
- Apache is an open source Web server that is distributed free.
- Apache runs on Unix-based operating systems (including Linux and Solaris) and Windows 98/NT/XP.

#### **WAMP**

- Windows, Apache, MySQL, and PHP -- a popular combination of software for use as a web server;
   Software for Microsoft Windows
- WAMPs are packages of independently-created programs installed on computers that use a Microsoft Windows operating system.
- A number of WAMP software exist for download. A convenient one is XAMPP.

#### Web security

- Backups are a way of securing information; they are another copy of all the important computer files kept in another location. These files are kept on hard disks, CD-Rs, CD-RWs, DVD, flash disks and tapes.
- Anti-virus software consists of computer programs that attempt to identify, thwart and eliminate computer viruses and other malicious software (malware).

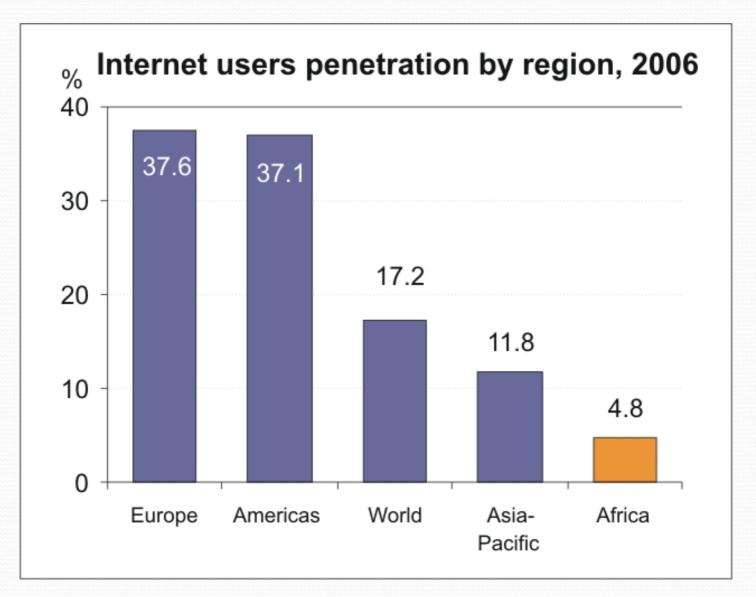
### Web Security

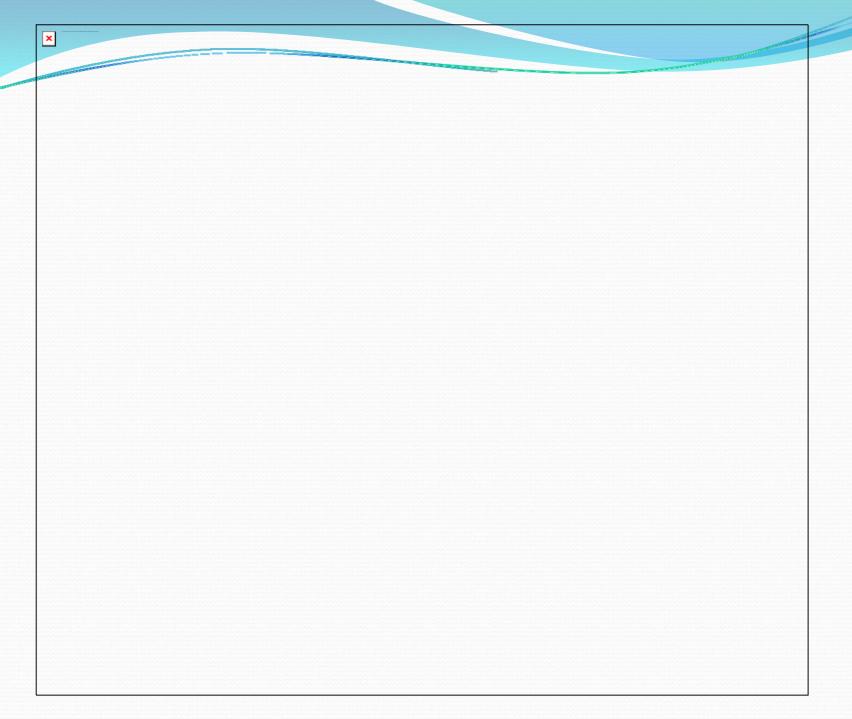
- Firewalls are systems which help protect computers and computer networks from attack and subsequent intrusion by restricting the network traffic which can pass through them, based on a set of system administrator defined rules.
- Access authorization restricts access to a computer to group of users through the use of authentication systems.

Data on ICT in Africa Updated: 24-04-2008

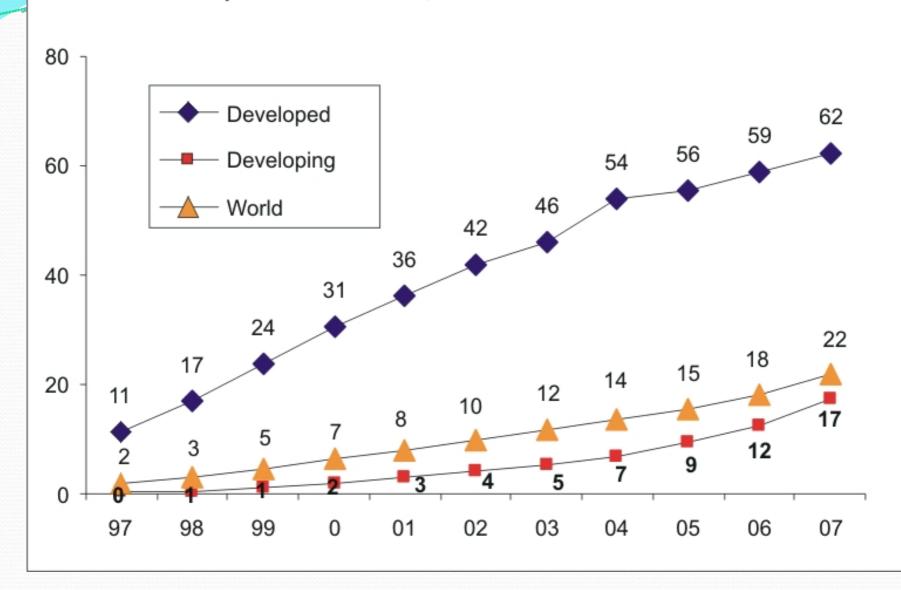
Source: ITU World Telecommunication/ICT Indicators

Database.



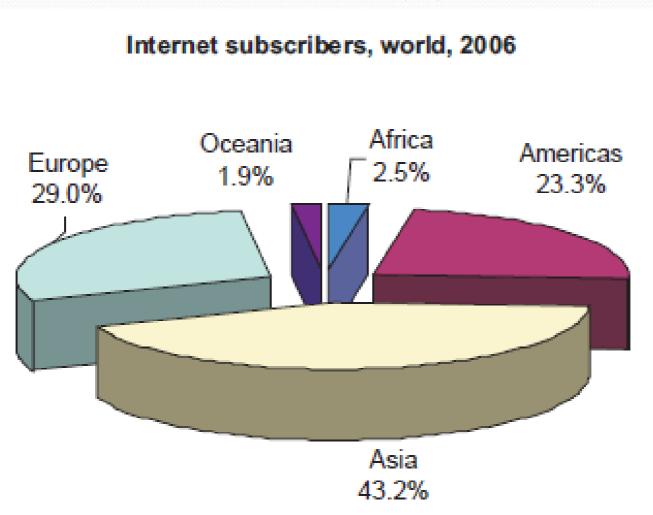


#### Internet users per 100 inhabitants, 1997-2007

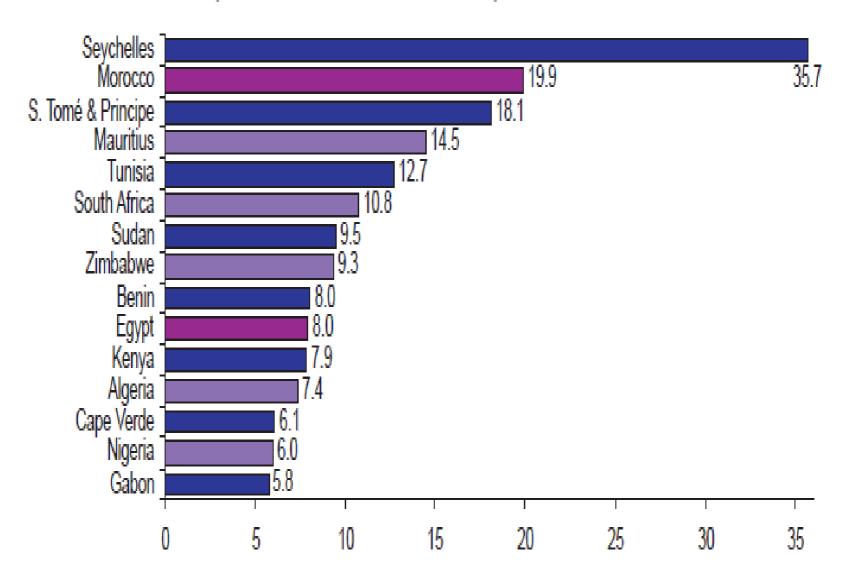


#### Where is Africa on the Net?

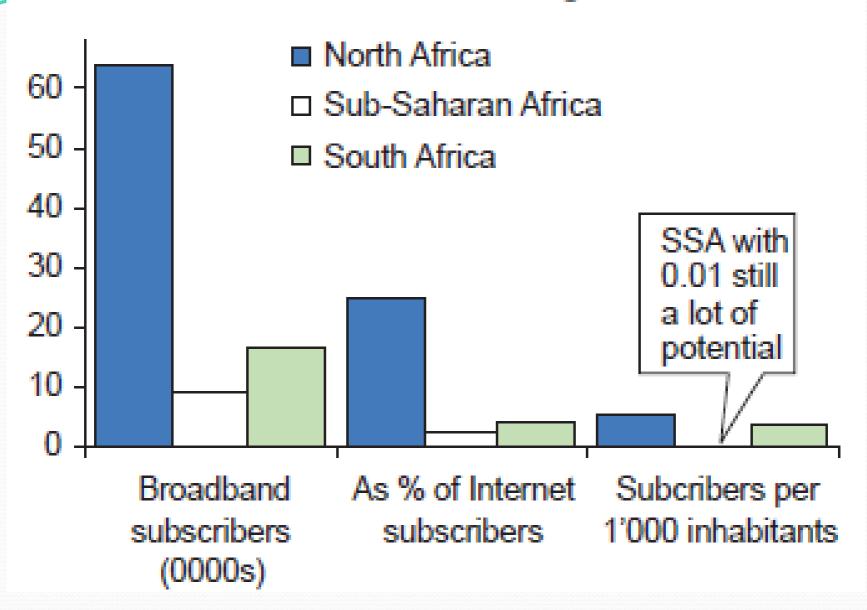
Source: ITU World Telecommunication/ICT Indicators (WTI) Database.

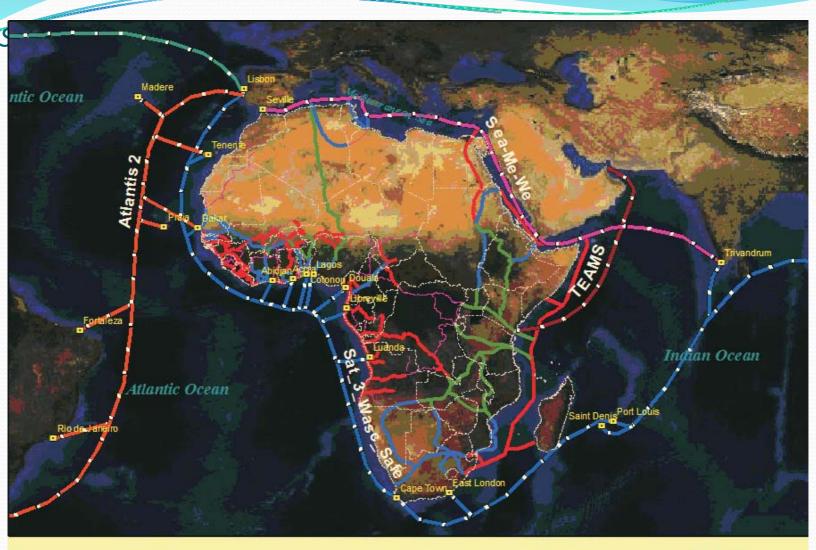


Top 15 African countries - Internet users per 100 inhabitants, 2006



### Broadband in African sub-regions, 2006





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### **Optical Fiber Network in Africa**



### **Experimental section**

- Creating a server using the available software
- Hardware requirements
- How to convert your computer to a server.
  - At least 512 MB RAM
  - Network card
  - At least 20GB hard disk space
  - Pentium 4 and above (e.g. dual core)

- Minimal computing knowledge is required to setup a webserver.
- A number of applications that are free for download are available for download. However, the best is XAMPP which installs Apache webserver, PHP server language and MySQL database on your computer, ready for use.

# Technology:

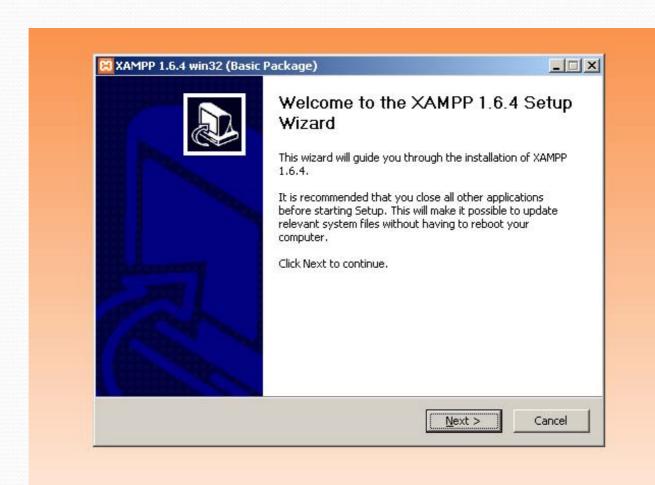
- Server software: XAMPP PHP, MySQl, Apache and Windows environment.
- An eight port switch it costs less than 1,400 (or \$20 USD) to buy one.
- A program known as PHP Generator for mySQL it generates scripts that will allow you to add, delete, update data on the database.

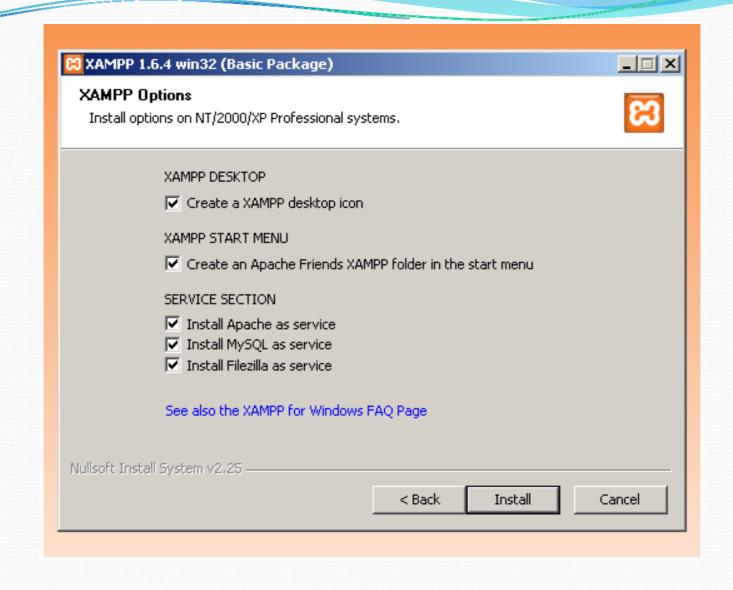
- Programs exist that allows users to edit or add data to mySQL database without knowledge of web programming.
- It is possible to for formulas to be put to other academics on the web within a local area network.

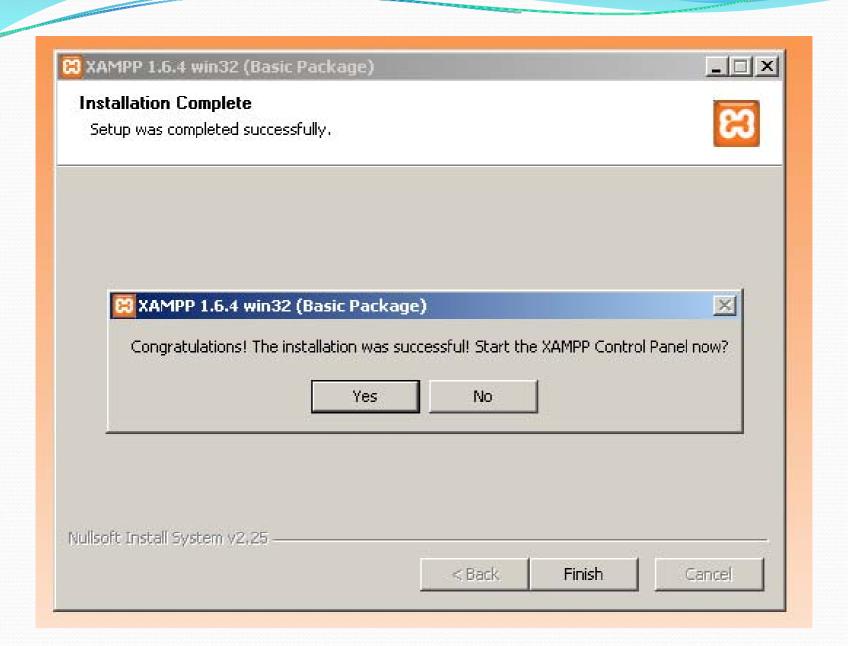
### Example: Setup of webserver using XAMPP

Download the latest installer













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# ICT chemistry applications

- Need to install macromedia software for editing WebPages
- Macromedia Suite installs Dreamweaver, Flash Macromedia among others

# Example of Flash macromedia

• robinson.html

## Other applications

- Creation of a toxic substances database.
- Online calculations which other scientists can access e.g. ..\..\xampp\htdocs\newzawadi2.html

### In summary

- Use of webserver can enhance your research.
- Colleagues and students can access your documents online (login access)
- Unless you put documents on the server site, no one will ever see them.

Thank you for listening