Mathematical Software I

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Outline

Computing

Consider computing in a broad sense - not just *Computer Science*

- Numerical computation (floating point, scientific)
- Discrete computation (integer, exact arithmetic)
- Symbolic computation
- Geometrical computation

Introduction Computer Performance Software and Documentation Licenses Application Software Software and OS Choices Virtu

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Computer Performance
Performance Measures

- Speed
  - Clock speed- MHz or GHz (megahertz or gigahertz; HZ, Hertz, cycles per second)
  - Computing speed - MFlops, GFlops, TeraFlops, or PetaFlops (floating point operations per second)
  - Communication bandwidth - Bus, switch, or interconnect bandwidth MB/s or GB/s (megabytes or gigabytes per second, bytes per second)
- Size
  - Number of processors or cores (processing units)
  - Cache size - MB, GB (megabytes, gigabytes)
  - Memory size - MB, GB (megabytes, gigabytes)
  - Disk size - MB, GB, or TB (megabytes, gigabytes, or terabytes)

History and Future of Computing

My personal experience...
Then (1990):

One 20MHz processor, 8MB memory, two 104MB disk drives, and a 3.5" 1.44MB floppy disk drive.

Now (2010):

Two 2.93GHz 6-core processors, 16GB memory, a 1TB disk drive, and a double layer DVD drive (approx. 8.5GB).

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History and Future of Computing

The future is now?
Now (2011):


Dual core 1GHz processor, 512MB memory, 16GB memory.

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Moore's Law

Named after Intel co-founder Gordon E. Moore states that the number of transistors on a given chip can be doubled every two years.

This has been the guiding principle of progress in electronics and computing since Moore first formulated the famous dictum in 1965.

Microprocessor Transistor Counts 1971-2011 & Moore's Law

Top 500

www.top500.org

The Top500 report lists the 500 fastest computer system being used today. In 1993 the collection was started and has been updated every 6 months since then. The best Linpack benchmark performance achieved is used as a performance measure in ranking the computers.

Supercomputer Performance
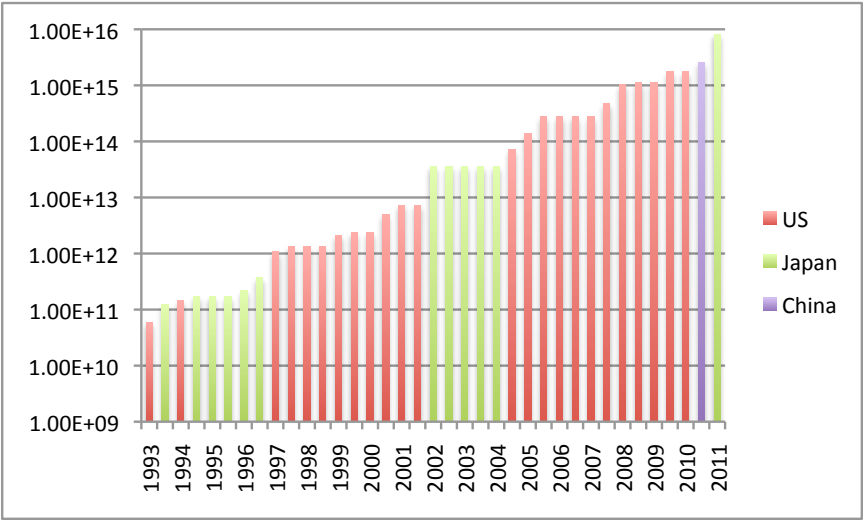
Software and Documentation Licenses

- Proprietary software
  - Protected by copyright, or trademark, owned, usage may be restricted by a license
- Free and Open Source software
  - Free as in beer
  - Free as in speech
- Copyright
  - Protected by copyright
- Creative Commons License
  - Can be reused, and incorporated into other work

Software and Documentation Licenses

Additional information:

- Free Software Foundation
  http://www.fsf.org
- GNU Project
  http://www.gnu.org
- Creative Commons
  http://creativecommons.org
- Electronic Frontier Foundation
  http://www.eff.org

Application Software

1. Computer Algebra Systems (CAS)
2. Numerical Computing Environment
3. Statistics Software
4. Typesetting Software

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Symbolic Computation

Symbolic Computation
Computer Algebra Systems

Proprietary

- Magma
- Maple
- Mathemetica
- MuPad (part of Matlab)

Symbolic Computation
Computer Algebra Systems

Open Source

- Axiom

- Maxima

- Sage http://www.sagemath.org

- Singular

- SymPy (and iPython) http://code.google.com/p/sympy (also
  see: http://www.python.org, http://www.scipy.org,
  http://ipython.scipy.org)

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Symbolic Computation

Symbolic Computation
Maple

- Symbolic algebra package
- Programming language
- "... environment of choice for scientific and engineering problem-solving, mathematical exploration, data visualization and technical authoring"

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Symbolic Computation
Maple

Introduction   Computer Performance   Software and Documentation Licenses   Application Software   Software and OS Choices   Virtu
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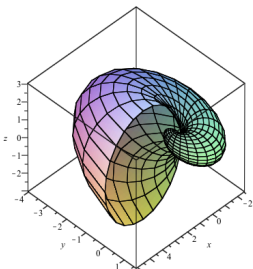
Symbolic Computation

Symbolic Computation
iPhone4s - Siri

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Numerical Computation
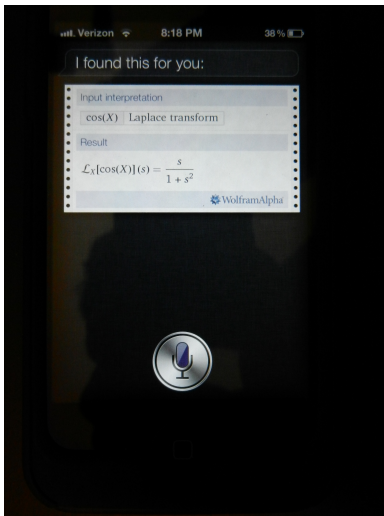
Numerical Computation

Proprietary

- Matlab

Open Source

- GNU Octave http://www.gnu.org/software/octave
- R http://www.r-project.org
- Scilab http://www.scilab.org
- SciPy http://www.scipy.org

Numerical Analysis Software
http://en.wikipedia.org/wiki/List_of_numerical_analysis_software

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Numerical Computation

Numerical Computation
MATLAB

- Matrix laboratory
- Programming language designed for mathematical computation, analysis, visualization, and algorithm development
- Integrated development environment
- Applications include: prototyping, garphics, data analysis, GUI development
- "MATLAB The Language of Technical Computing"
- "MATLAB and companion toolboxes provide engineers, scientists, mathematicians, and educators with an environment for technical computing applications"

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Numerical Computation

Numerical Computation
MATLAB

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Numerical Computation

Statistics Software

Proprietary

- Matlab
- Minitab
- SAS
- SPSS

Open Source

- R http://www.r-project.org

Statistics Software http://en.wikipedia.org/wiki/Statistics_software

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Typesetting and Presentation

Typesetting and Presentation
TₑX/LᴬTₑX

TₑX

- **TₑX** - created by Donald E. Knuth
- It is a markup language (typesetting language), in fact a programming language
- TₑX (doesn't create an image) it is a page description
- Designed to create beautiful mathematics documents (papers, books)
- In the public domain, cross platform, very powerful, complicated, not WYSIWYG (for the most part)

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Typesetting and Presentation

Typesetting and Presentation
TeX/LaTeX

LaTeX

- **LaTeX** - created by Leslie Lamport
- LaTeX is a comprehensive set of markup commands (macros) used with the typesetting program TeX
- In the public domain, cross platform
- Simplify the use of TeX

The Comprehensive TeX Archive Network http://www.ctan.org
The TeX Users Group http://www.tug.org

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Typesetting and Presentation

Typesetting and Presentation
TEX/LATEX Add-Ons

- Persentations, colors, transitions
- Output formats pdf, ps
- Graphics
- Charts, tables, and diagrams
- Processors, viewers/previewers, and front-ends, device drivers
- Style files, journal specific style files, book publishers
- Environments
  - **TEXShop** - http://pages.uoregon.edu/koch/texshop
  - **TEXWorks** - http://tug.org/texworks
- Bibliographic Database Managers
  - **BibDesk** - http://bibdesk.sourceforge.net
  - **JabRef** - http://jabref.sourceforge.net

Introduction   Computer Performance   Software and Documentation Licenses   Application Software   Software and OS Choices   Virtu

Typesetting and Presentation

Typesetting and Presentation

TeXShop

Introduction   Computer Performance   Software and Documentation Licenses   Application Software   Software and OS Choices   Virtu

Typesetting and Presentation

Typesetting and Presentation

Bibliographic Database Manager - BibDesk

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Typesetting and Presentation

OS and Software Choices

> ### Guiding principle
>
> Whenever possible I will use FOSS software and documentation that is governed by the CC license, or similar

- Operating System - Linux (Ubuntu)
- Virtual Machine - VirtualBox
- Software - Python and other FOSS packages

Virtual Machine

A virtual machine (VM) is a software implementation of a machine
(i.e. a computer) that executes programs like a physical machine.
Modern virtual machines are implemented with either software
emulation or hardware virtualization.
http://en.wikipedia.org/wiki/Virtual_machine

VirtualBox

VirtualBox is a powerful x86 and AMD64/Intel64 virtualization product.

VirtualBox allows an unmodified operating system with all of its installed software to run in a special environment, on top of your existing operating system. This environment, called a *virtual machine*, is created by the virtualization software by intercepting access to certain hardware components and certain features. The physical computer is then usually called the *host*, while the virtual machine is often called a *guest*. Most of the guest code runs unmodified, directly on the host computer, and the guest operating system *thinks* it's running on real machine.

http://www.virtualbox.org/wiki

VirtualBox

VirtualBox runs on Windows, Linux, Macintosh, and Solaris hosts and supports a large number of guest operating systems including but not limited to Windows (NT 4.0, 2000, XP, Server 2003, Vista, Windows 7), DOS/Windows 3.x, Linux (2.4 and 2.6), Solaris and OpenSolaris, OS/2, and OpenBSD.

VirtualBox
VirtualBox Manager

VirtualBox
Linux in VirtualBox
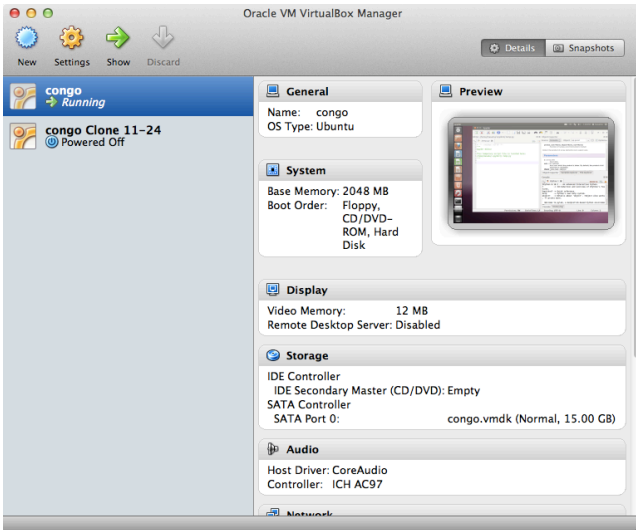
Linux

Linux is a computer operating system which is based on free and open source software. Although many different varieties of Linux exist, all are Unix-like and based on the Linux kernel, an operating system kernel created in 1992 by Linus Torvalds.

Linux can be installed on a wide variety of computer hardware, ranging from mobile phones, tablet computers, routers and video game consoles, to desktop computers, mainframes and supercomputers. Linux is a leading server operating system, and runs most of the fastest supercomputers in the world.
http://en.wikipedia.org/wiki/Linux

Python

Python is a powerful dynamic programming language that is used
in a wide variety of application domains. Key features include:

- clear, readable syntax
- strong introspection capabilities
- intuitive object orientation
- natural expression of procedural code
- full modularity, supporting hierarchical packages
- exception-based error handling
- very high level dynamic data types
- extensive standard libraries and third party modules for
  virtually every task
- extensions and modules easily written in C, C++ (or Java for
  Jython, or .NET languages for IronPython)
- embeddable within applications as a scripting interface

http://www.python.org/about

Software Installation and Configuration

- VirtualBox - install VirtualBox and Oracle VM VirtualBox Extension Pack
  http://www.virtualbox.org/wiki/Downloads
- Create a VM image (virtual disk image; USB or hard drdive)
- Configure VirtualBox
- Create a shared folder
- Start virtual machine, create user, and use