

Mathematical Software I

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 - Symbolic Computation
 - Numerical Computation
 - Typesetting and Presentation
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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

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).

History and Future of Computing

The future is now?

Now (2011):



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

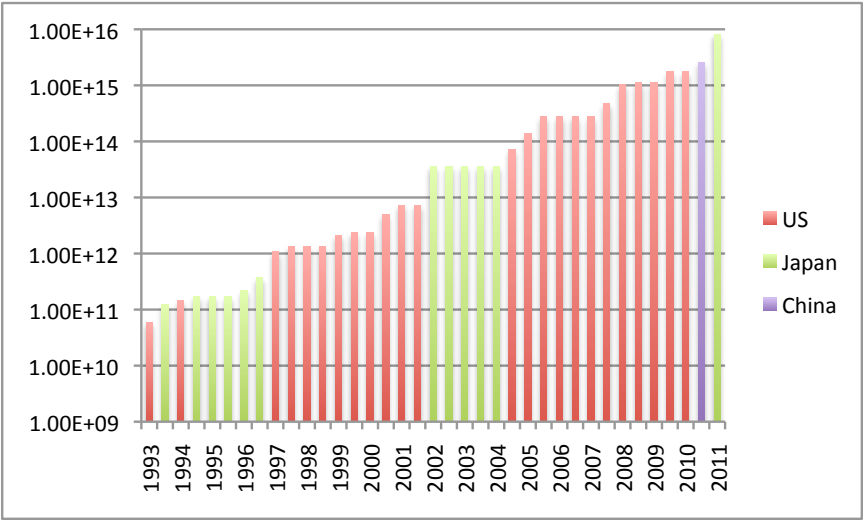
Top 500



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

Symbolic Computation

Computer Algebra Systems

Proprietary

- Magma
- Maple
- Mathematica
- 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>)

Symbolic Computation

Maple

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

Symbolic Computation

Symbolic Computation

Maple

untitled

Text Math Drawing Plot Animation Hide

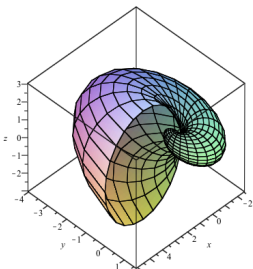
45 45 0

$\int (\sin(x)^2 + x^3, x);$

$$-\frac{1}{2} \sin(x) \cos(x) + \frac{1}{2} x + \frac{1}{4} x^4 \quad (1)$$

with(plots):

sphereplot $\left(\left(\frac{4}{3} \right)^{\text{theta}} \cdot \sin(\text{phi}), \text{theta} = -1 .. 2 \cdot \text{Pi}, \text{phi} = 0 .. \text{Pi} \right)$



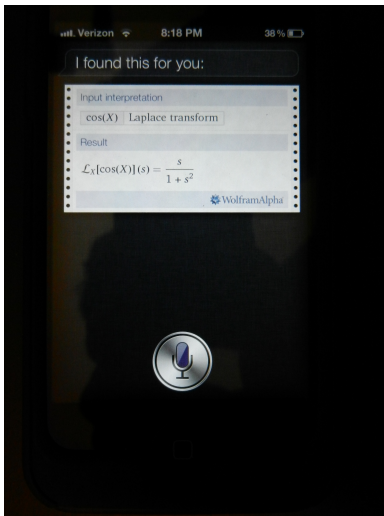
Ready

Server: 1 Memory: 0.68M Time: 0.08s Text Mode

Symbolic Computation

Symbolic Computation

iPhone4s - Siri



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

Numerical Computation

MATLAB

- Matrix laboratory
- Programming language designed for mathematical computation, analysis, visualization, and algorithm development
- Integrated development environment
- Applications include: prototyping, graphics, 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”

Numerical Computation

Numerical Computation

MATLAB

The image displays the MATLAB 7.10.0 (R2010a) environment. The interface includes a File Explorer on the left showing the 'Current Folder' with files like 'heat2d.m'. The Command Window shows the execution of the 'heat2d' function, resulting in a 1x11 double array. The Workspace window shows the 'ans' variable. The bottom-left pane shows the MATLAB script for 'heat2d.m', which calculates the heat diffusion in a slab. The bottom-right pane shows a 3D surface plot of the results, titled 'Figure 1', illustrating the temperature distribution over a 2D domain.

Command Window Output:

```
>> heat2d
ans =
columns 1 through 4
0 0.100000000000000 0.200000000000000 0.300000000000000
columns 5 through 8
0.400000000000000 0.500000000000000 0.600000000000000 0.700000000000000
columns 9 through 11
0.800000000000000 0.900000000000000 1.000000000000000
```

Figure 1: Heat diffusion in a slab

The 3D surface plot shows a temperature distribution over a 2D domain. The vertical axis represents temperature, ranging from 0 to 100. The horizontal axes represent spatial coordinates, ranging from 0 to 1. The surface is colored with a gradient from blue (low temperature) to red (high temperature), showing a peak in the center of the domain.

Script Editor (heat2d.m):

```
36
37     alphax = K*dt/dx^2;
38     alphay = K*dt/dy^2;
39
40     for k=1:n
41         for j=2:m
42             for i=2:l
43                 u(i,j,k+1) = alphax*u(i-1,j,k) + (1 - 2*alphax - 2*alphay)*u(i,j,k)
44                     + alphax*u(i+1,j,k) + alphay*u(i,j-1,k) + alphay*u(i,j+1,k);
45             end
46         end
47     end
48     save h1.mat
```

Statistics Software

Proprietary

- Matlab
- Minitab
- SAS
- SPSS

Open Source

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

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

Typesetting and Presentation

T_EX/L^AT_EX

T_EX

- **T_EX** - created by Donald E. Knuth
- It is a markup language (typesetting language), in fact a programming language
- T_EX (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)

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>

Typesetting and Presentation

T_EX/L^AT_EX Add-Ons

- Presentations, 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
 - **T_EXShop** - <http://pages.uoregon.edu/koch/texshop>
 - **T_EXWorks** - <http://tug.org/texworks>
- Bibliographic Database Managers
 - **BibDesk** - <http://bibdesk.sourceforge.net>
 - **JabRef** - <http://jabref.sourceforge.net>

Typesetting and Presentation

Typesetting and Presentation
T_EXShop

The image shows a LaTeX Beamer presentation window with two panes. The left pane displays a slide titled "Numerical Computation" with the subtitle "MATLAB". The slide content includes a list of bullet points:

- Matrix laboratory
- Programming language designed for mathematical computation, analysis, visualization, and algorithm development
- Integrated development environment
- Applications include: prototyping, graphics, 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"

The right pane shows the source code for the presentation, which is a LaTeX Beamer document. The code includes various Beamer commands such as `\begin{frame}`, `\begin{itemize}`, `\item`, `\end{itemize}`, `\end{frame}`, `\begin{block}`, and `\end{block}`. It also includes navigation commands like `\backslash`, `\forward`, `\up`, `\down`, `\leftarrow`, `\rightarrow`, `\search`, and `\refresh`. The code is numbered from 414 to 464.

Typesetting and Presentation

Typesetting and Presentation

Bibliographic Database Manager - BibDesk

The screenshot shows the BibDesk application window titled "SteadyPE.bib". The interface includes a menu bar with "Action", "New", "Edit", "Delete", and "TeX Preview". A search bar labeled "Search Bibliography" is present. The main window is divided into a left sidebar and a main content area.

Left Sidebar:

- GROUPS: Lib... (41)
- EXTERNAL: Web (Empty)
- SMART
- STATIC
- KEYWORDS: Em... (41)

Main Content Area:

Keyword	BibTeX	Cite Key	Title
article	Phillips2008		A coupling of mixed and continuous Galerkin...
book	Renardy2004		An Introduction to Partial Differential Equations
article	Roose2003		Solid stress generated by spheroid growth estim...
article	Shi1999		W^2, p regularity of the displacement problem...
article	Showalter2...		Diffusion in poro-elastic media
techre...	Showalter2...		Partially saturated flow in a poroelastic medium
article	Showalter2...		Diffusion in deforming porous media
techre...	Smillie2004		A hydro-elastic model of hydrocephalus
article	Steck2000		A finite difference model of loadinduced fluid di...
book	Wang2000		Theory of Linear Poroelasticity with Applications...
techre...	Zeng2000		A poroelastic model for acoustic landmine detection
article	Zienkiewicz...		Dynamic behavior of saturated porous media: th...

Selected Entry Details (Showalter2003):

Diffusion in deforming porous media (article)

Author: Showalter, R. E.

Journal: Dyn. Contin. Discrete Impuls. Syst. Ser. A Math. Anal.

Year: 2003

Volume: 10

Number: 5

Pages: 661--678

100%

41 publications

Drop Files Here

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.

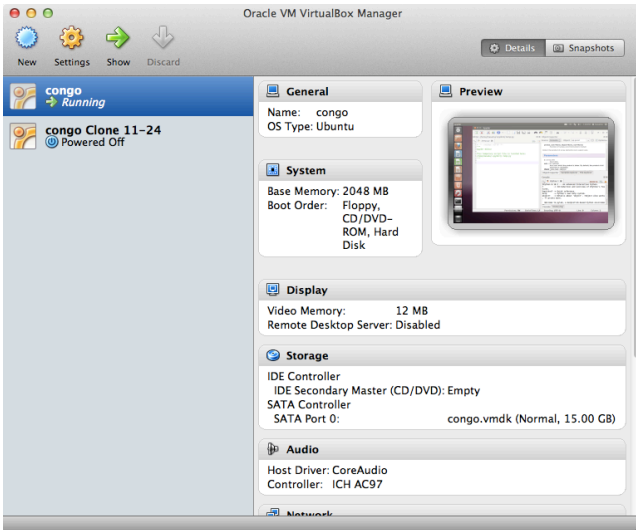
<http://www.virtualbox.org/wiki>

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



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 drive)
- Configure VirtualBox
- Create a shared folder
- Start virtual machine, create user, and use