

# Scientific Tools for Linux

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# Goals

## » Goals

Mathematical Tools

Electrical Engineering Tools

Chemistry Tools

Physics Tools

Other Tools

Questions?

This presentation is intended to introduce you to the vast array of software available for scientific applications that run on Linux. Software is available for electrical engineering, mathematics, chemistry, physics, biology, and other fields.

# Non-Free Mathematical Tools

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Mathematical Tools

» Non-Free Mathematical Tools

» MATLAB

» Mathematica

» Maple

» Free Mathematical Tools

» GNU Octave

» mathomatic

» R

» SAGE

Electrical Engineering Tools

Chemistry Tools

Physics Tools

Other Tools

Questions?

- MATLAB (MathWorks)
- Mathematica (Wolfram Research)
- Maple (Maplesoft)
- S-Plus (Mathsoft)

# MATLAB

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Electrical Engineering Tools

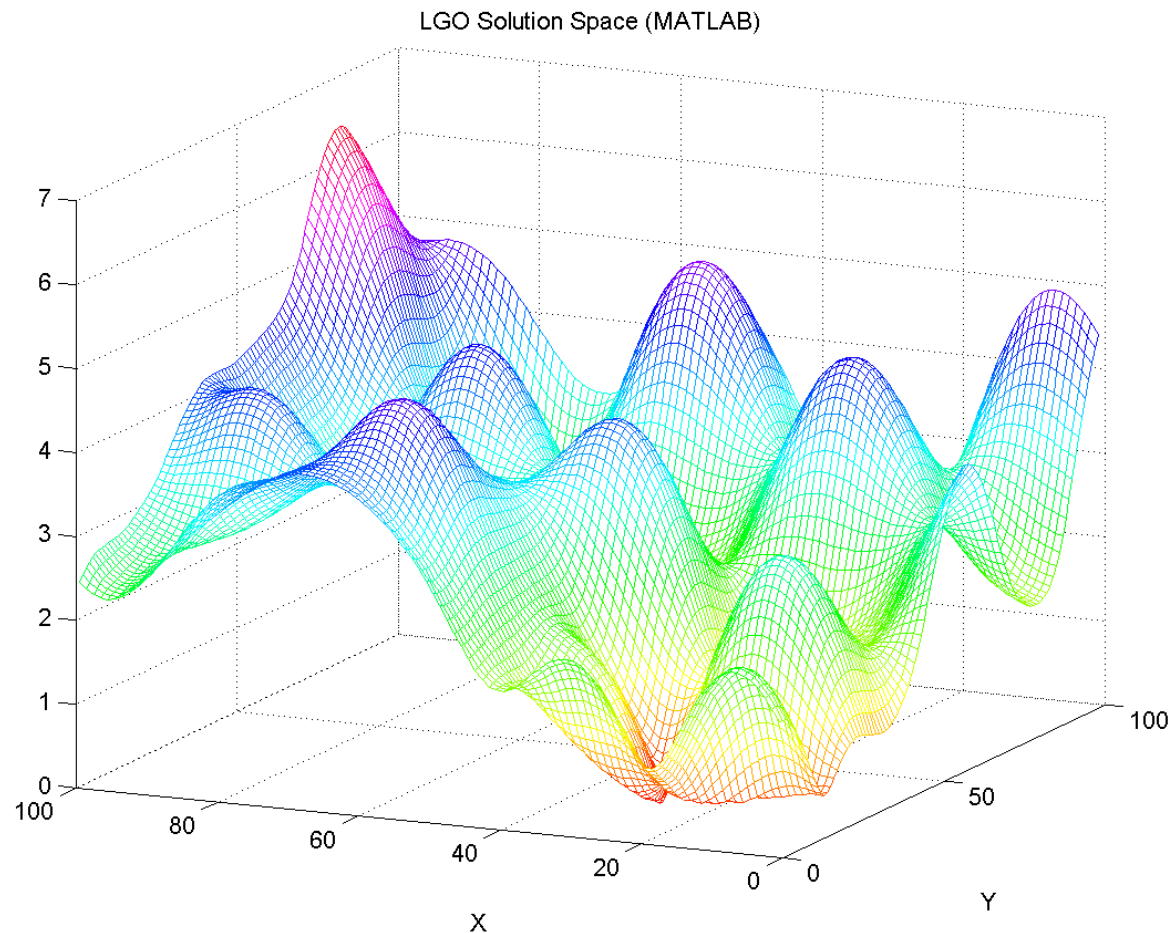
Chemistry Tools

Physics Tools

Other Tools

Questions?

- MATLAB is a fully functional mathematics language
- You may be familiar with it from use in classes



# Mathematica

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Electrical Engineering Tools

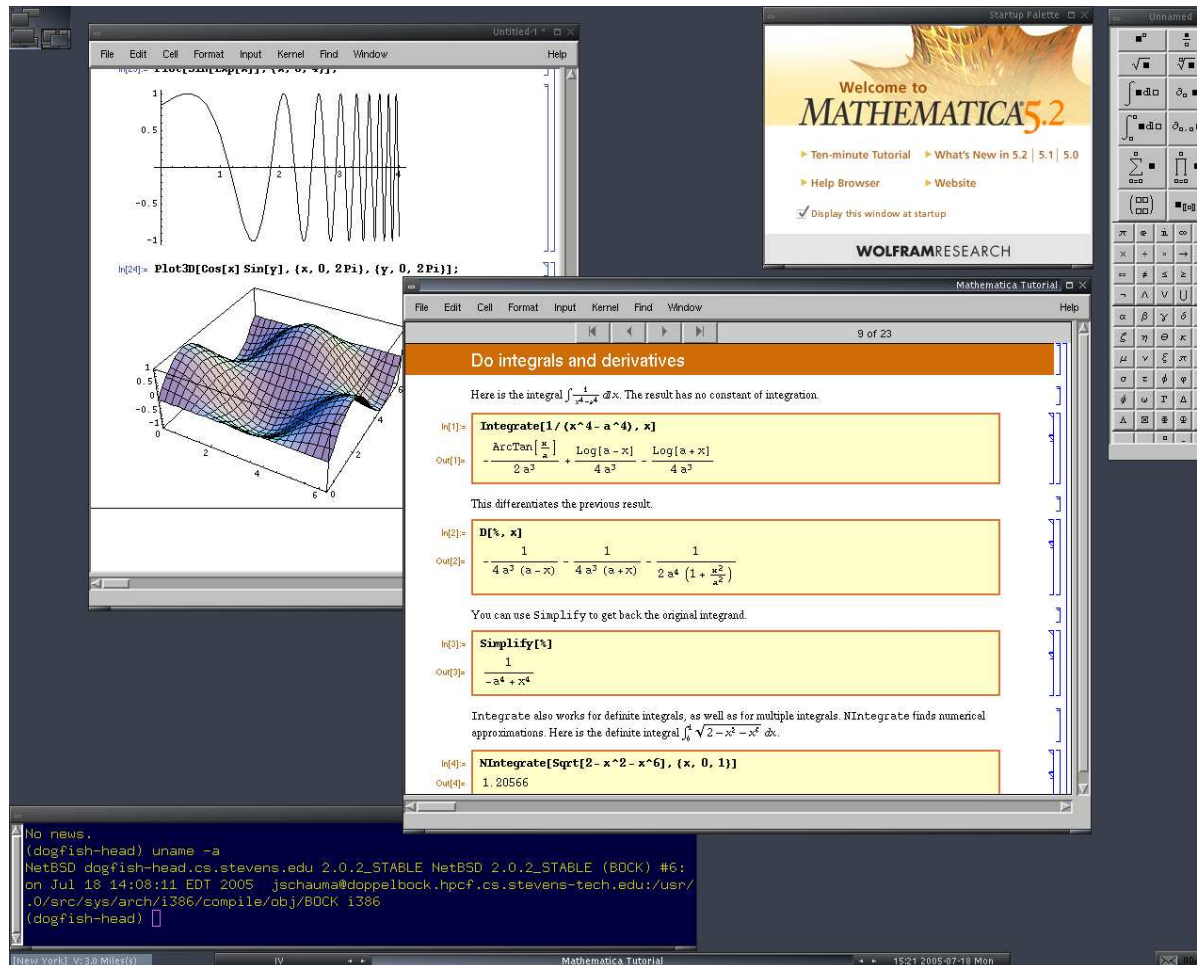
Chemistry Tools

Physics Tools

Other Tools

Questions?

- Worksheet-based mathematics suite
- Linux versions can be buggy and bugfixes can be slow



# Maple

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Electrical Engineering Tools

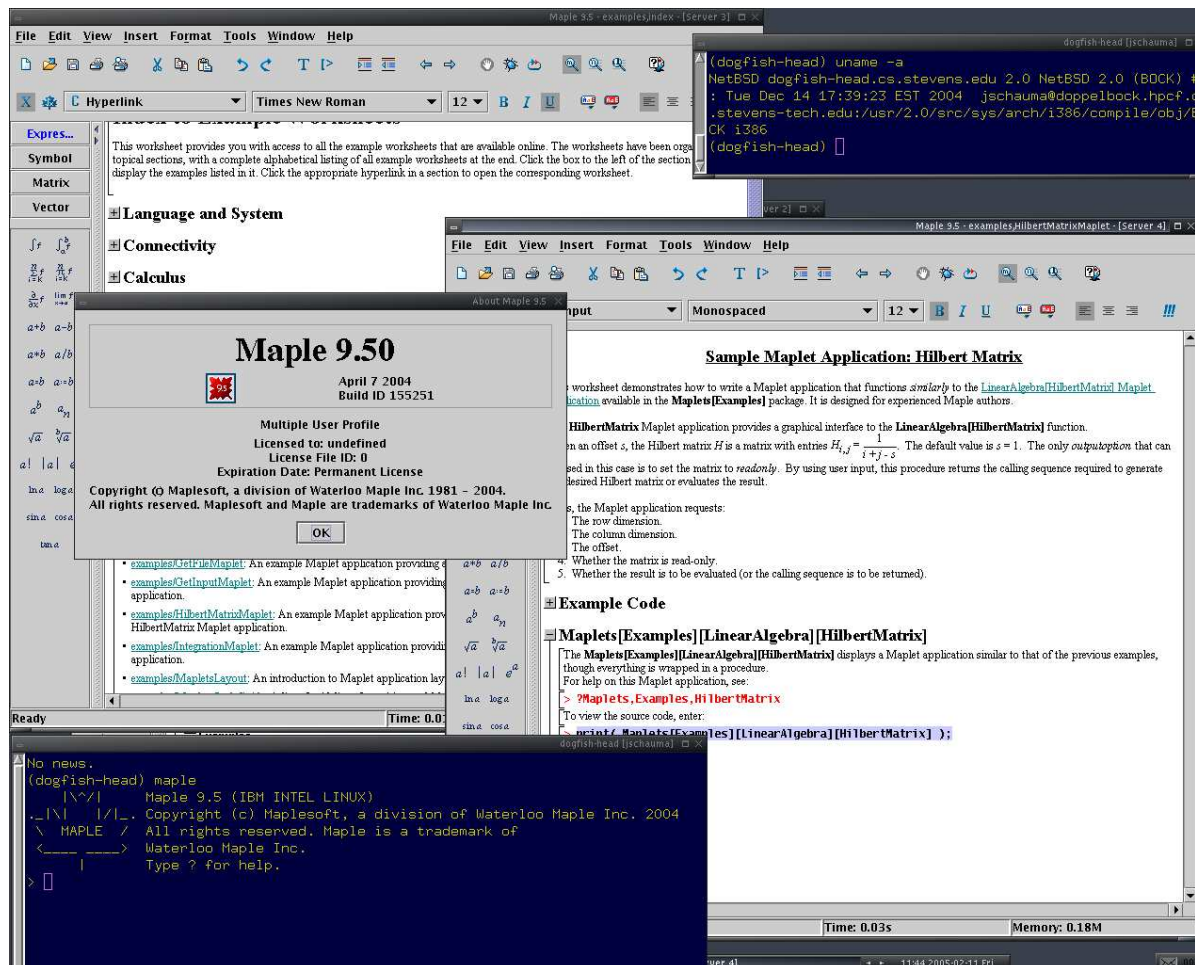
Chemistry Tools

Physics Tools

Other Tools

Questions?

- Large mathematics suite
- GUI mode and CLI mode available



# Free Mathematical Tools

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Other Tools

Questions?

- GNU Octave: MATLAB clone
- mathomatic: automatic algebraic manipulator
- R: environment for statistical analysis
- SAGE: open source mathematics toolkit

# GNU Octave

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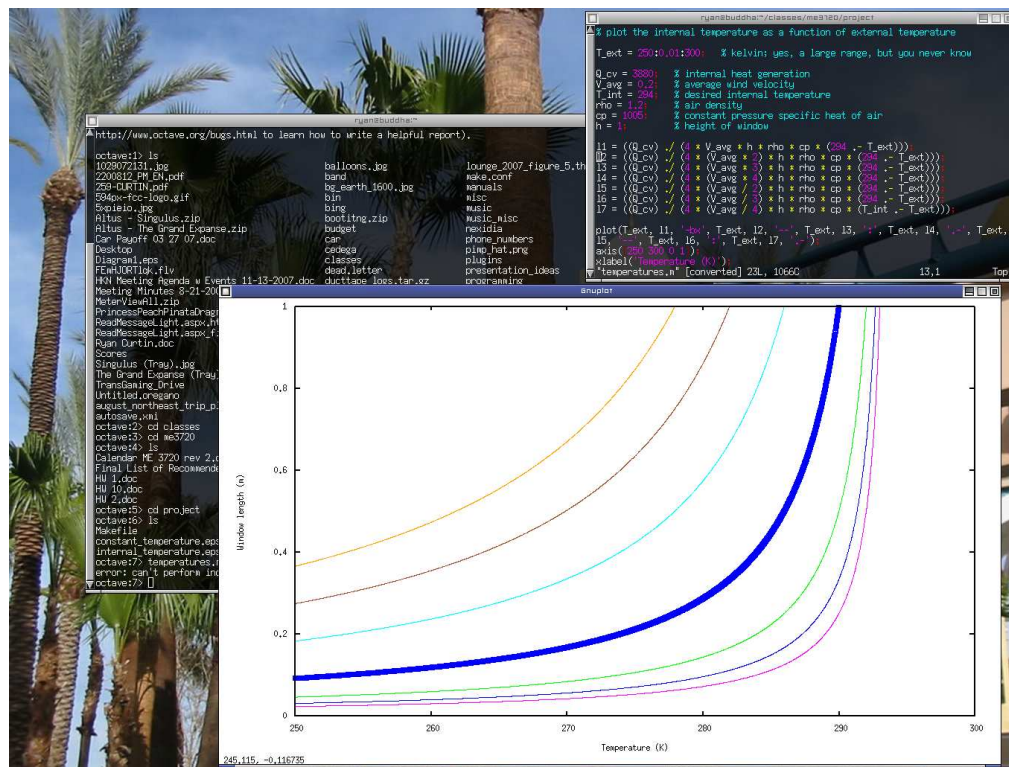
Chemistry Tools

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Other Tools

Questions?

- Open-source clone of MATLAB
- MATLAB compatibility is mostly implemented, but differences still exist
- Uses gnuplot for graphing



# mathomatic

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Other Tools

Questions?

- Command-line algebraic manipulator
- Solves systems of equations quickly
- Very colorful output

# R

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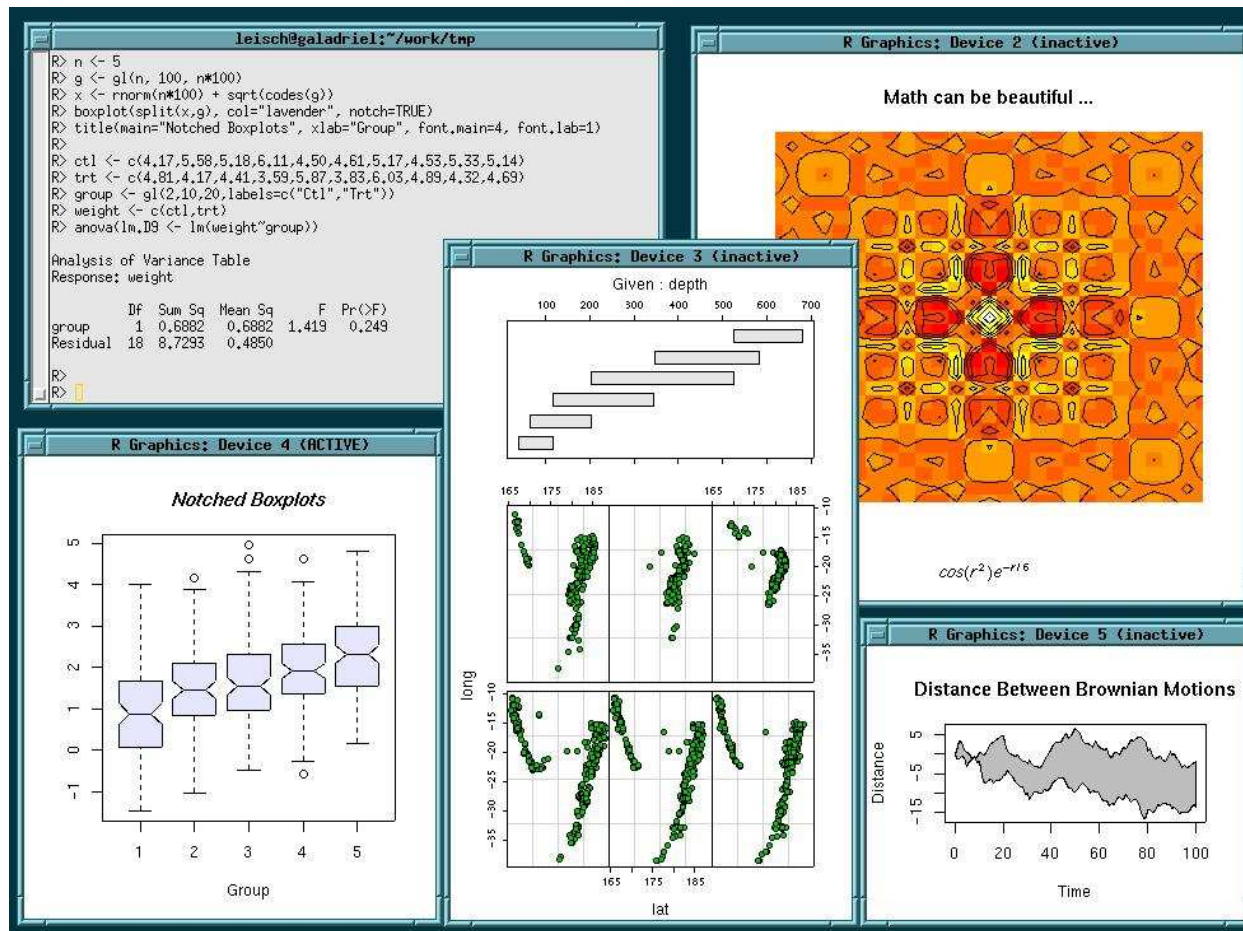
Chemistry Tools

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Other Tools

Questions?

- Open-source clone/derivative of S-Plus
- Statistical analysis suite



# SAGE

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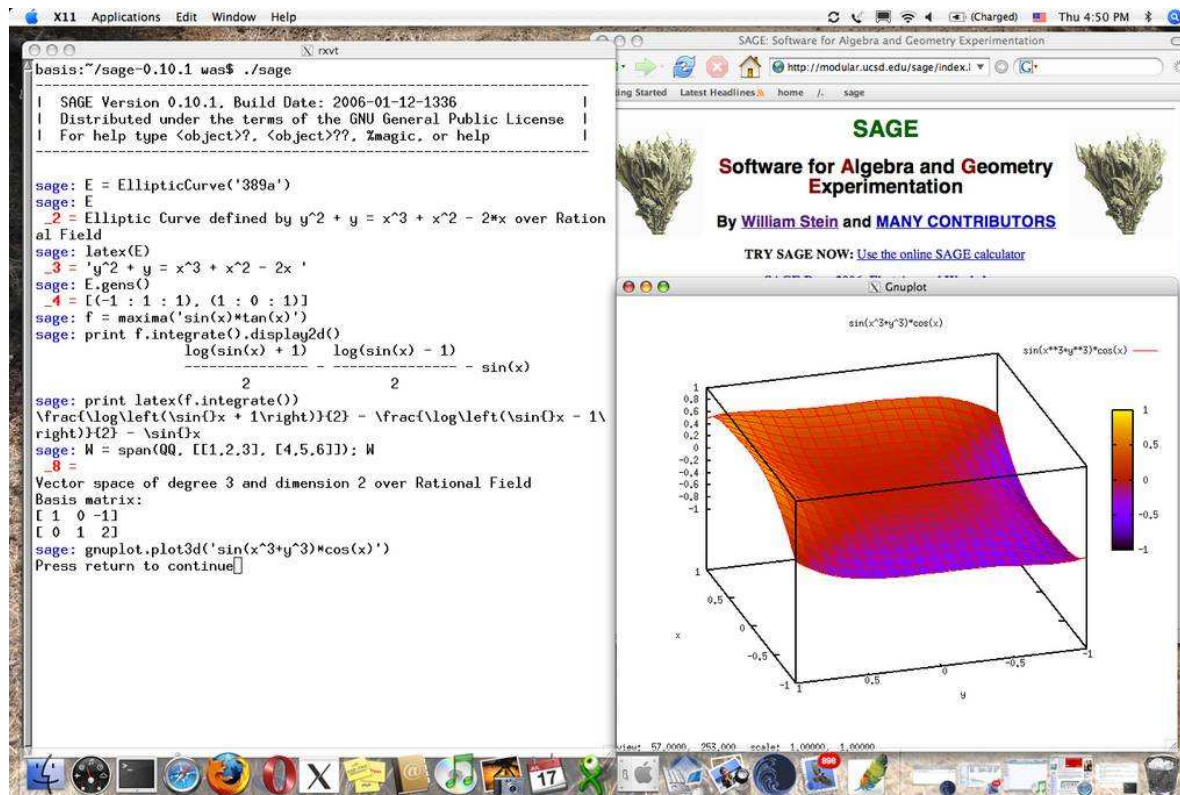
Chemistry Tools

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Other Tools

Questions?

- A "viable free open source alternative to Magma, Maple, Mathematica, and Matlab"
- Modular: you can call other programs from inside SAGE
- Uses Python for mathematics



# Non-free EE tools

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» Free EE tools

» ngspice

» gnucap

» ktechlab

» gEDA: Introduction

» gEDA: Workflow

» ghdl

» iverilog

» GPL Cver

» gtkwave

» gwave

» gspeakers

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Questions?

- **ModelSim**: highly advanced digital circuit simulator
- **Cadence Virtuoso**: IC development suite
- **Altera Quartus**: HDL synthesis/simulation design tool
- **Xilinx ISE**: HDL-based design tool for Xilinx FPGAs

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Chemistry Tools

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Questions?

- **ngspice, gnuicap**: backend circuit simulators
- **ktechlab**: fledgling GUI schematic input project
- **gEDA**: fully-featured electronics design automation suite
- **ghdl, freehdl**: VHDL compilers and simulators
- **iverilog, GPL Cver**: Verilog compiler and simulator
- **gtkwave**: Waveform viewer
- **gwave**: Waveform viewer for SPICE-like simulations
- **gspeakers**: Speaker enclosure design tool

# ngspice

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Questions?

- SPICE simulator with graphing support
- Uses 'spice' as a backend
- Uses gnuplot as a graphing frontend
- Default library does not contain very many devices
- `http://ngspice.sourceforge.net/`

# gnucap

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Questions?

- GNU Circuit Analysis Package: general purpose circuit simulator
- Not like SPICE: designed to do true mixed-mode simulation (analog/digital)
- Mostly compatible with the SPICE language
- Command-line tool for use in batch mode, like SPICE variants
- <http://www.gnu.org/software/gnucap/>

# ktechlab

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Questions?

- Digital/analog circuit simulator for basic to moderately complicated circuits
- Relatively new; version 0.3.6 is the most recent
- Similar in design to Cadence PSpice or NI Multisim (Windows-only products)
- Does not seem to have specific models of devices
- Library of generic devices seems somewhat limited, but useful for basic applications
- <http://ktechlab.org/>

# gEDA: Introduction

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Questions?

- gEDA is the most prominent suite of electronic design automation tools
- A massive set of applications with functionality including:
  - Schematic capture
  - Attribute management
  - Bill of materials (BOM) generation
  - Netlisting
  - Analog/digital simulation
  - PCB layout
- <http://www.geda.seul.org>

# gEDA: Workflow

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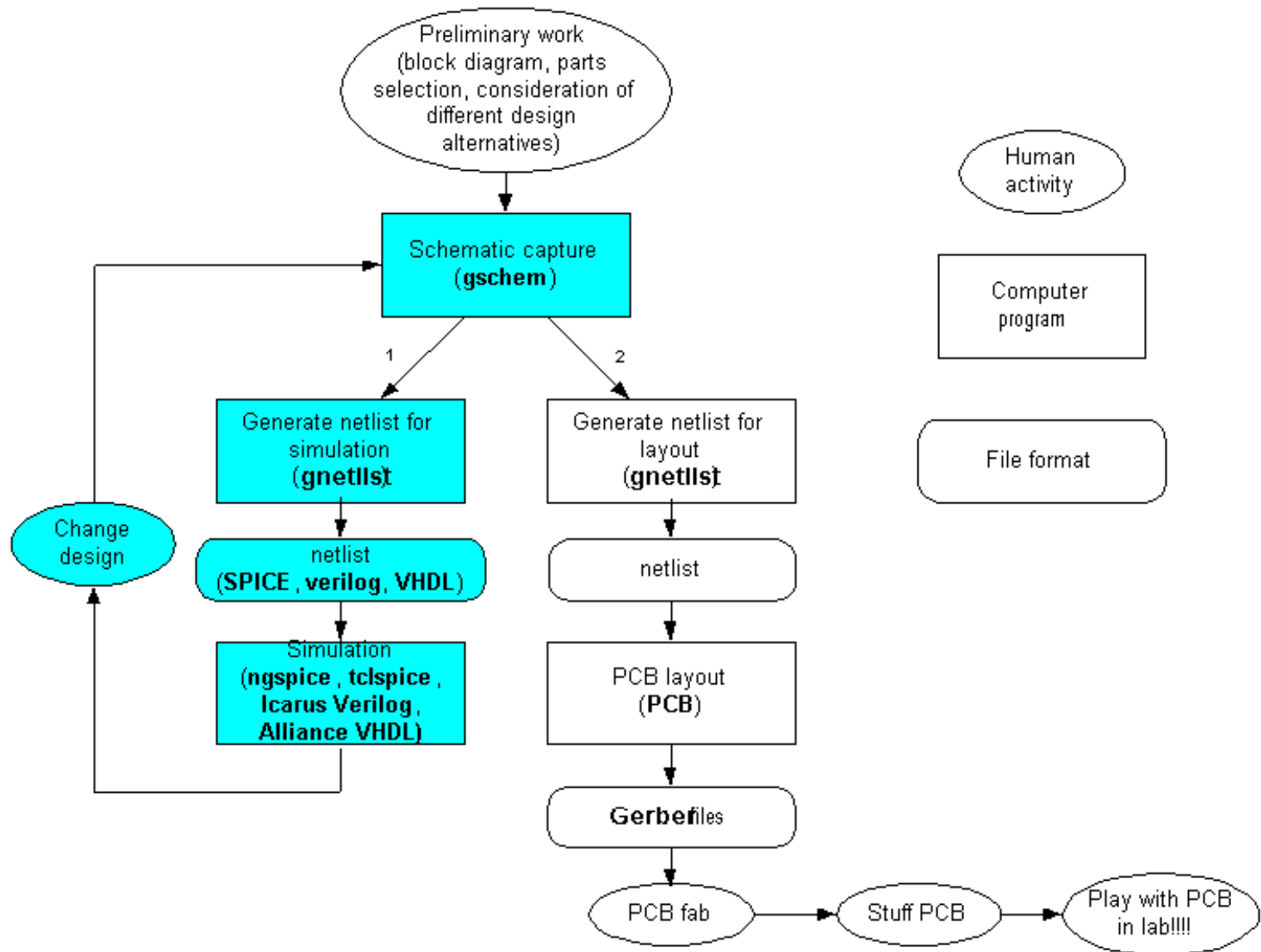
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Questions?

Ryan Curtin



# ghdl

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Questions?

- Complete VHDL simulator that implements the IEEE VHDL standard
- Does not support Verilog
- Mostly compatible with ModelSim
- Does not support synthesis
- Runs from the command line; use gtkwave to look at simulation results
- Slow development: last release (0.26) in April 2007
- <http://ghdl.free.fr/>
  
- freehdl is a similar project that never got off the ground
- <http://freehdl.seul.org/>

# iverilog

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Questions?

- Verilog simulation and synthesis (to XNF files) implemented
- One-man design team (Steven Williams), so releases are slow
- Project is currently relatively stable
- <http://www.icarus.com/eda/verilog/>

# GPL Cver

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Questions?

- Fully implemented 1995 P1364 Verilog HDL simulator
- Does not do synthesis
- Has been around for longer than iverilog and has a larger design team
- Releases are very slow since the project became proprietary
- New project is 'CVC'; but is non-free
- <http://www.pragmatic-c.com/gpl-cver/>

# gtkwave

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Questions?

- GTK-based application for viewing digital waveforms
- Reads many different simulation formats: LXT, LXT2, VZT, GHW, VCD, EVCD
- Simple, stable (current version is 3.1.3), and easy to use
- Configurable through rc files
- <http://home.nc.rr.com/gtkwave/>

# gwave

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Questions?

- A waveform viewer for analog waveforms, such as SPICE output
- Can read output from HSpice, Spice2, Spice3, ngspice, CAzM, gnucap, and other binary / ASCII formats
- A component of the gEDA suite
- Relatively stable; last release 2006-06-06
- <http://www.geda.seul.org/tools/gwave/>

# gspeakers

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Chemistry Tools

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Other Tools

Questions?

- Simple GTK-based application for speaker design
- Development appears to have stopped; last version (0.11) released in 2004
- Driver design, enclosure design, and crossover network design
- Sometimes confusing and unpolished, but somewhat usable
- Has the potential to be a great application for speaker design... if someone finished it
- <http://gspeakers.sourceforge.net/>

# Chemistry tools

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» Chemistry tools

» chemtool

» rasmol / pymol

» easychem

» openbabel

Physics Tools

Other Tools

Questions?

- **chemtool**: organic molecule drawing program
- **rasmol, pymol**: molecular renderer
- **easychem**: presentation-focused chemical structure drawing program
- **openbabel**: converter for molecular modeling file formats
- <http://sal.jyu.fi/Z/2/index.shtml> lists many chemistry programs for Linux

# chemtool

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Physics Tools

Other Tools

Questions?

- A small program for drawing chemical structures
- Uses GTK
- Stable; latest release 1.6.11
- Produces simple, functional chemical structures
- Exports eps for easy inclusion in  $\text{\LaTeX}$  documents
- <http://ruby.chemie.uni-freiburg.de/~martin/chemt>

# rasmol / pymol

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Physics Tools

Other Tools

Questions?

- Molecule analyzers: makes molecules easier to visualize and interpret
- RasMol can convert between various color palettes for easy interpretation, but its power is mostly from the fairly simple command-line interface
- PyMol produces images that are usually found on textbook covers or pages due to their intricate detail
- PyMol does not have as powerful a command-line interface as RasMol
- RasMol: <http://www.openrasmol.org/>
- PyMol: <http://pymol.sourceforge.net/>

# easychem

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Physics Tools

Other Tools

Questions?

- Simple program designed to draw chemical molecules
- Still in semi-early development: current version is 0.6 and a new version has not appeared since early 2006
- <http://easychem.sourceforge.net/>

# openbabel

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Physics Tools

Other Tools

Questions?

- A suite of several programs including conversion utilities, a 'grep' for molecules, and other tools

- Converts over 80 different chemistry-related formats

- [http://openbabel.sourceforge.net/wiki/Main\\_Page](http://openbabel.sourceforge.net/wiki/Main_Page)

# Physics Tools

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» Physics Tools

» ROOT

» lightspeed

» Open Dynamics Engine

» celestia

Other Tools

Questions?

- **ROOT**: large-scale data analysis tool
- **lightspeed**: interactive OpenGL relativistic simulator
- **jaxodraw**: Java program for drawing Feynman diagrams
- **Open Dynamics Engine**: industrial quality libraries for articulated rigid body dynamics simulations
- **celestia**: OpenGL 3D space simulator
- **maestro**: NASA's program to control the Spirit and Opportunity rovers

# ROOT

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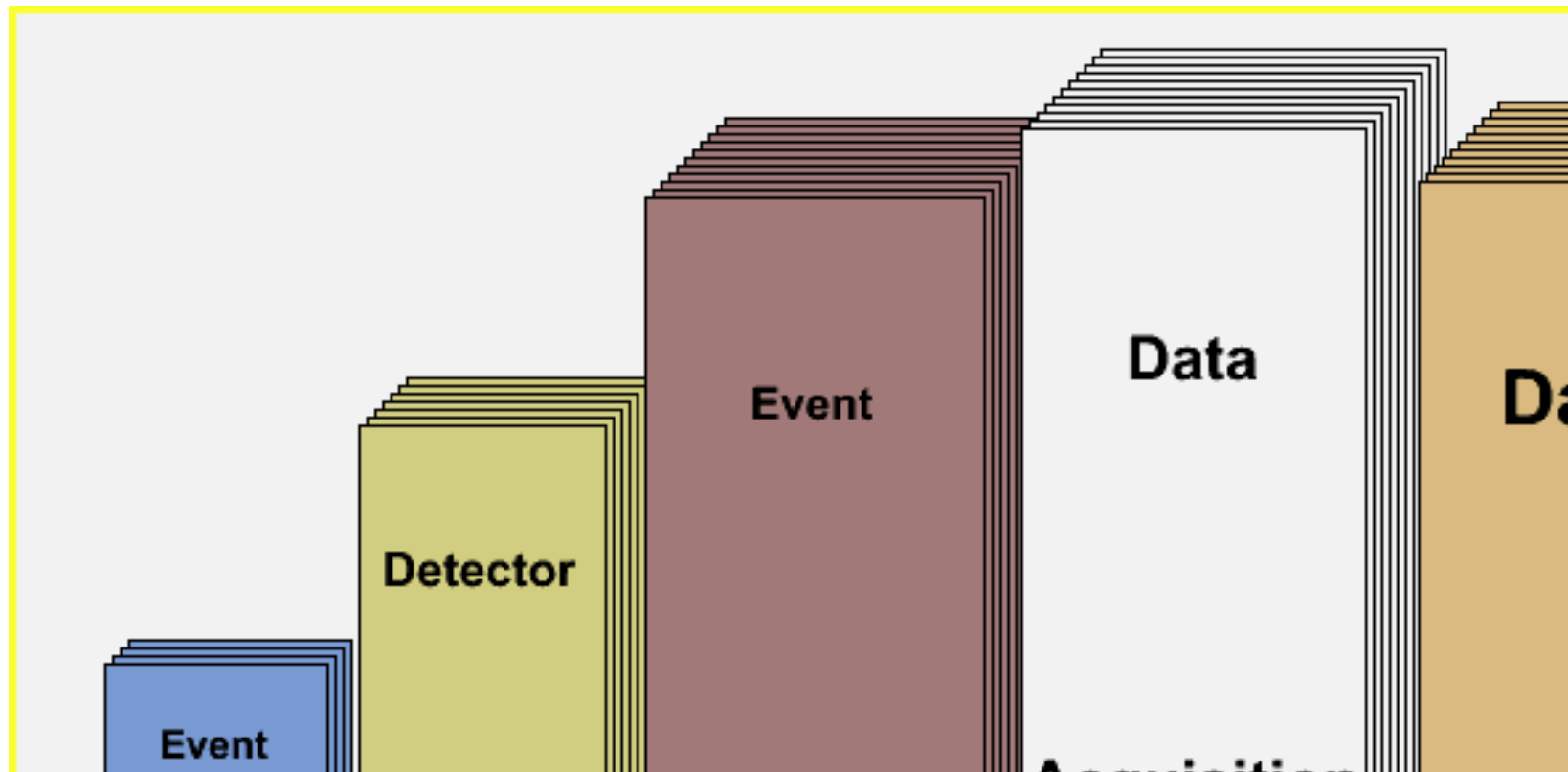
» Open Dynamics Engine

» celestia

Other Tools

Questions?

- A set of object-oriented frameworks for processing very large sets of data
- Designed for parallel operation on clustered systems
- The language ROOT uses is C++
- <http://root.cern.ch/>



# lightspeed

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Other Tools

Questions?

- Simple utility for viewing relativistic effects on geometric lattices
- Can handle 3DStudio and LightWave 3D objects
- Uses OpenGL to render objects
- For a given velocity, this utility displays what it would look like when relativistic effects are considered

# Open Dynamics Engine

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Other Tools

Questions?

- Free physics SDK licensed under the BSD license
- Used by many non-mainstream games, including smash hits like **Amsterdam Taxi Madness**, **Simulator Bob**, and **Shanghai Street Racer**
- Good for simulating *articulated* rigid body structures
- Emphasizes speed and stability over physical accuracy
- <http://www.ode.org/>

# celestia

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Other Tools

Questions?

- OpenGL 3D space simulation
- Not technically a physics tool, but it's really cool
- Allows you to explore space, with nice OpenGL graphics
- `http://www.shatters.net/celestia/`

# Other tools

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Other Tools

» Other tools

» dia

» kivio

» L<sup>A</sup>T<sub>E</sub>X

» xfig

» umbrello

Questions?

- **dia**: Diagram drawing utility
- **kivio**: KOffice flowcharting utility (similar to Visio)
- **L<sup>A</sup>T<sub>E</sub>X**: typesetting utility
- **xfig**: Drawing utility
- **The GIMP**: GNU Image Manipulation Program
- **umbrello**: UML modeler

# dia

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» Other tools

» dia

» kivio

»  $\LaTeX$

» xfig

» umbrella

Questions?

- GTK-based diagram drawing utility
- GUI model similar to the GIMP
- Can be used for flowcharting, circuit diagrams, block diagrams, and other diagrams
- Large database of components you can diagram and link together
- Exports as almost any graphics format
- <http://www.gnome.org/projects/dia/>

# kivio

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» dia

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»  $\LaTeX$

» xfig

» umbrello

Questions?

- KOffice's diagramming and flowcharting application
- Library of diagrammable components is not very large; however, it supports Dia components
- Very similar to Dia, but GUI model is like KOffice and not the GIMP
- <http://www.koffice.org/kivio/>

- Typesetting language; able to produce beautiful documents
- Used to make this presentation
- See previous presentations on L<sup>A</sup>T<sub>E</sub>X:  
<http://lugatgt.org/articles/latex2/>
- <http://www.latex-project.org>

# xfig

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»  $\LaTeX$

» xfig

» umbrello

Questions?

- Tool for drawing complex diagrams
- Similar to Dia and Kivio, but GUI is different
- <http://www.xfig.org>

# umbrello

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» xfig

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Questions?

- Qt-based UML modeler
- Can take a series of C files and generate a UML hierarchy
- Somewhat buggy for very large diagrams
- <http://uml.sourceforge.net/>

# Questions?

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