# Overview of software packages and capabilities

Lecture 2

Special Topics:
Device Modeling

---

# Introduction

- Semiconductor device modeling
  - 1-D vs 2-3-D problems
- Circuit modeling, device modeling in 2-D
- Modeling of radiation transport
- Common coupled problems in physics and engineering (electric/magnetic fields, heat transport, etc.)

---

# Outline

- AMPS-1D: photovoltaic devices; other junctions
- SCAPS: photovoltaic devices; radiation detectors can be modeled through a special approach
- PSPICE: electrical circuit design
- MCNP: Monte Carlo radiation transport
- COMSOL Multiphysics: partial differential equation solver

---

# AMPS-1D

- A one-dimensional device simulation program for the Analysis of Microelectronic and Photonic Structures (AMPS)
- Created by the group at the Center for Nanotechnology Education and Utilization, the Pennsylvania State University (professor Stephen J. Fonash and his group)
- The program is continuously supported and further developed (http://www.ampsmodeling.org)
- Originally created for Unix, now under Windows platform (for Windows 7 runs under XP mode/Virtual PC)
- YouTube tutorial: https://youtu.be/9jhs-UFZ_ZM

---

# AMPS-1D

- The objective of AMPS is to teach how material properties (e.g., band gap, affinity, doping, mobilities, doping, gap state defect distributions in the bulk and at interfaces, etc.) and device design/structure together control device physics and thereby device response to light, voltage, and temperature
- Numerically solves for 1-D case the three governing semiconductor device equations (Poisson equation, and free electron and hole continuity equations)

---

# AMPS-1D: modeled structures

- Homojunction and heterojunction p-n and p-i-n, solar cells, detectors, microelectronic (ME) structures (e.g., MIS, FET)
- Multi-junction solar cell and ME structures
- Compositionally-graded detector, solar cell, and ME structures
- Schottky barrier devices with optional back layers
- Novel device ME, photovoltaic, and opto-electronic structures

## AMPS-1D main features

- Able to handle various defect levels and doping, energy gap and special energy distributions
- Shockley-Read-Hall (S-R-H) and band-to-band recombination (no tunneling)
- Boltzmann and Fermi-Dirac statistics
- Varying material properties
- Very general treatment of contacts
- Ability to handle transport in devices under voltage bias, light bias, or both

## AMPS-1D input

- Device is represented as a stack of layers with specified material properties (semiconductor, metal, or insulator) and interface parameters
- All input parameters fall into one of three general categories:
  - Parameters that apply over the entire device
  - Parameters that apply to a particular region
  - Parameters that define the illuminating spectrum (for cases with light).

## AMPS-1D output

- Developed standard models, at the level of best efficiencies for major PV devices (Si, CdTe, CIGS)
- Capable of calculating:
  - band diagrams
  - current components, current-voltage characteristics
  - recombination, generation profiles
  - electric field as a function of light intensity, voltage, temperature
- Output: plots of the above functions

## AMPS-1D: recent developments

- New wxAMPS is available through university of Illinois (Angus Rockett group)
- Executable and supporting files for Windows 7/8
- Beyond the original AMPS kernel, wxAMPS incorporates two tunneling models
- Based on the option for an unlimited number of layers in the simulation, modeling graded solar cells can be implemented easily in wxAMPS

Y. Liu, Y. Sun, and A. Rockett, "A new simulation software of solar cells--wxAMPS", Solar Energy Materials and Solar Cells, 2012.

## SCAPS-1D

- SCAPS (a Solar Cell Capacitance Simulator) is a one-dimensional thin-film solar cell simulation program
- Developed at the Department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium
- The program is continuously supported and further developed (http://scaps.elis.ugent.be)
- Runs under later Windows (7/8)

## SCAPS-1D

- Originally was developed for polycrystalline cell structures of the $CuInSe_2$ and the CdTe family
- Recent developments make it applicable to crystalline and amorphous solar cells (Si, GaAs, a-Si)
- The basic equations are: the Poisson equation, relating the charge to the electrostatic potential $\Phi$, and the continuity equations for electrons and holes (same as AMPS-1D)

## SCAPS-1D: input

- Device is represented as a stack of layers, up to 7 semiconductor layers with specified properties
- Almost all parameters can be graded (i.e. dependent on the local composition or on the depth in the cell, can be entered from a file)
- Recombination mechanisms: band-to-band (direct), Auger, SRH-type
- Contacts: specified work function or flat-band; optical property (reflection of transmission filter) filter

## SCAPS-1D: input

- Defect levels: in bulk, or at interface; various energy distributions and charge states (now including multivalent and metastable)
- Tunneling: intra-band tunneling (within a conduction band or within a valence band); tunneling to and from interface states
- Generation: either from internal calculation under illumination or from user supplied g(x) file (allows for modeling of radiation detectors)

## SCAPS-1D: output

- Working point for calculations: voltage, frequency, temperature
- Calculates energy bands, concentrations and currents at a given working point, *J-V* characteristics, AC characteristics (capacitance, conductance as function of *V* and/or *f* ), spectral response (also with bias light or voltage)
- Batch calculations possible; presentation of results and settings as a function of batch parameters

## SCAPS-1D: output

- In each calculation the running parameter (V, f, or $\lambda$) is varied in the specified range
- Plot all calculated parameters, such as I/V, C/V, C/f, Q($\lambda$), band diagrams, concentrations, and currents
- All calculations can be saved in ASCII format
- When divergence occurs, the points calculated so far are not lost, they are shown on the corresponding graphs

## SCAPS-1D additional features

- Data analysis is supported within the package: any ASCII-text file can be read as a measurement file
  - The file extension indicates which kind of measurement it contains: '.iv', '.cv', '.cf' or '.qe'
- A built-in curve fitting facility
- Quantum efficiency panel
- A panel for the interpretation of admittance measurements (C/f and C/V)

## Other device simulation packages

- TCAD - Technology Computer Aided Design –is a branch of electronic design automation that models semiconductor fabrication, and operation
- The modeling of the fabrication is termed Process TCAD, while the modeling of the device operation is termed Device TCAD
- May also include compact models (such as the well known SPICE transistor models), which try to capture the electrical behavior of such devices

## Other device simulation packages

- Major suppliers of TCAD tools include Synopsys, Silvaco, Crosslight, Cogenda Software, VisualTCAD and Global TCAD Solutions
- The open source GSS, Archimedes, Aeneas, NanoTCAD ViDES, DEVSIM, and GENIUS have some of the capabilities of the commercial products
- TCAD Central (http://www.tcadcentral.com/) maintains an information resource for available TCAD software, both commercial and free

## SPICE: history

- SPICE program (Simulation Program with Integrated Circuit Emphasis) is dedicated to process modeling in electrical circuits
- First SPICE program was developed at the Electronics Research Laboratory of the University of California, Berkeley (SPICE1 1973, SPICE2 1975, coded in Fortran), was distributed for a nominal charge to cover cost of magnetic tapes
- SPICE inspired and served as a basis for many other circuit simulation programs

## SPICE: general capabilities

- AC/DC analysis
- DC transfer curve analysis (a sequence of nonlinear operating points calculated while sweeping an input voltage or current)
- Noise analysis
- Transfer function analysis (a small-signal input/output gain and impedance calculation)
- Transient analysis (time-domain large-signal solution of nonlinear differential algebraic equations)

## SPICE: available packages

- XSPICE, academic spinoff, by Georgia Tech
- Cider (previously CODECS, from UC Berkeley/ Oregon State Univ.), added semiconductor device simulation
- HSPICE, commercial product by Synopsys, Inc.
- PSPICE, commercial product, presently owned by Cadence, distributed under OrCad
- Several SPICE-based circuit simulation programs by various IC manufacturers

## OrCAD package: Capture CIS

- Capture CIS (component information system) - used to create schematics and produce connectivity and simulation information for printed circuit boards (PCB) and programmable logic designs
  - Choose to set up a PSpice project, PCB project, or programmable logic project when start a new project
- Provides standard libraries of parts that can be used to design schematics; use the property editor to add, change, or delete properties, create your own custom parts and library

## OrCAD package: Capture CIS

- The circuit diagram drawn in Capture is represented as a netlist of all the components and their respective connections to other components
- Text file can be parsed, properties of components modified before running through PSpice
- Multiple on-line tutorials are available (some are excessive in showing how to use every menu item)

## OrCAD package: Capture CIS

**Full schematic view**          **Editing part properties**
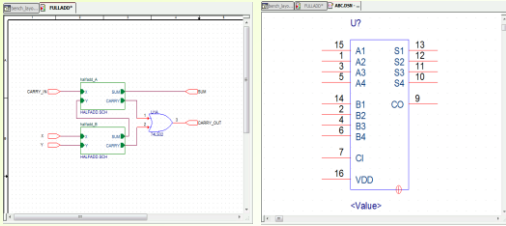


## OrCAD package: PSpice

- Pspice is a simulation tool that performs analysis of analog and mixed-signal circuits
- Includes model libraries that feature over 15,000 analog and 1,600 digital models of devices manufactured world-wide
- Uses schematics from Capture, including edited standard and custom parts
- Types of analyses: transient, AC, DC, parametric sweep, and worst-case

## OrCAD package: PSpice

- Advanced Analysis tool (used in conjunction with PSpice A/D) is available to analyze
  - Sensitivity – identifies critical circuit components
  - Optimizer – optimizes key circuit components
  - Monte Carlo – analyzes statistical circuit behavior and yield
  - Smoke – detects component stress
  - Parametric Plotter – examines solution space through nested sweeps

## OrCAD package: PSpice

- DC bias point analysis calculates node voltages and currents through devices in the circuit
- It takes into account any voltage sources applied to the circuit and any initial conditions set on devices or nodes in the circuit
- The output file provides a list of the entire analog and digital node voltages, currents, and other relevant parameters

## OrCAD package: PSpice

**Sample RC circuits for transient analysis**          **Waveform for voltage across capacitor**
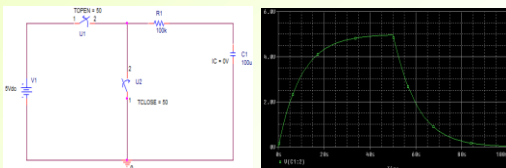


## MCNP

- Monte Carlo N-particle radiation transport package
- Developed and maintained by Los Alamos National Laboratory
- Neutron/Photon/Electron particle transport, including coupled transport
- General 3D geometry including array features
- Time dependent problems

## MCNP

- Various tally options and arrangements
- Many variance reduction techniques
- Calculations can be parallelized, and configured in a multiprocessing mode on a cluster of workstations (with PVM or MPI software)

## MCNP:
## Basic application areas

- Radiation dosimetry
- Radiation shielding design
- Health Physics
- Nuclear physics
  - Criticality Evaluations
  - Reactor Analysis and Design
- Any other problems dealing with ionizing radiation in the keV-MeV-GeV energy range

## MCNP:
## Medical physics applications

Examples discussed in MCNP Med. Phys. primer
- Calculation of dose from Tc-99m diagnostic therapy
- Calculation of Medical Internal Radiation Dose (MIRD), specific absorbed fraction (SAF) values using the ORNL MIRD phantom
- X-ray phototherapy effectiveness
- Prostate brachytherapy lifetime dose calculations
- A radiograph of the head using the Zubal head phantom

## MCNP:
## Medical physics applications

MIRD12 phantom
- ORNL 1996
- 35 discrete cells
- 3 materials (soft, bone, lung)
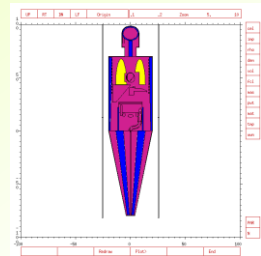


## MCNP:
## Medical physics applications

Zubal head phantom
- 85 x 109 x 120 voxels
- 2.2 x 2.2 x 1.4 mm3
- 25 Brain structure tallies
- 15 materials
- Jeff Evans, Ohio State
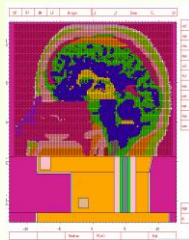


## COMSOL Multiphysics

- Partial differential equation solver package with front-end developed for visual input and output
- Takes input in terms of user-defined equations
- Most used through different "modules" with predefined "physics", greatly simplifying modeling of device geometry, governing equations, boundary conditions, etc.
- Available across platforms (Windows, MAC, Linux); since version 5 allows for creating physics-based apps

## COMSOL: Physics-based modeling (main program)

- Electrostatics, and electric currents
- Heat transfer in solids and fluids
- Joule heating
- Laminar flow
- Pressure acoustics
- Solid mechanics
- Transport of diluted species
- Additional physics interfaces through *modules*

## COMSOL Multiphysics: modules



## COMSOL Multiphysics: modules



## COMSOL: Geometry modeling

- Primitive solid objects, including block, cone, cylinder, sphere, ellipsoid, torus; parametric helix, curves and surfaces
- Interpolation curves; extrude, revolve, sweep; boolean operations union, intersection, difference, and partition
- Hybrid modeling with solids, surfaces, curves, and points
- Work Plane with 2D geometry modeling
- CAD import and interoperability with add-on CAD Import Module and LiveLink products for CAD
- CAD repair and defeaturing with add-on CAD Import Module and LiveLink products for CAD

## COMSOL: Meshing

- Free tetrahedral meshing
- Swept mesh with prism and hex elements
- Boundary layer meshing
- Free triangular meshing of 3D surfaces and 2D models
- Mapped and free quad meshing of 3D surfaces and 2D models
- Copy mesh operation; virtual geometry operations
- Mesh partitioning of domains, boundaries, and edges

## COMSOL: Results

- Visualization: surface plots, isosurface plots, arrow plots, slice plots, streamline plots, contour plots
- Post-processing
  - Integration, average, max, and min of arbitrary quantities over volumes, surfaces, edges, and points
  - Custom mathematical expressions including field variables, their derivatives, spatial coordinates, time, and complex-valued quantities
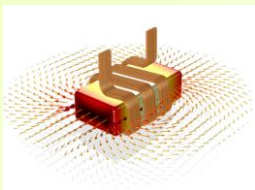
## COMSOL Multiphysics
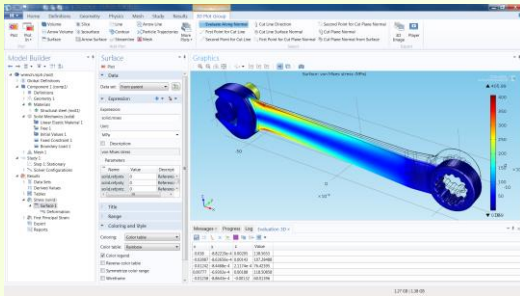


## COMSOL Multiphysics
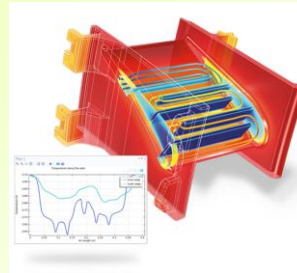


Example:
Stator blade in the turbine stage of a jet engine is heated by combustion gases, where the resulting temperature gradients introduce significant stresses.
To prevent the stator from melting, air is passed through a cooling duct in the blade.

## COMSOL: AC/DC module



COIL MODELING: The model shows a 50-Hz AC coil wound around a ferromagnetic core. The complex coil winding geometry can be easily modeled using a multiturn coil feature. Visualization shows the magnetic flux density (arrow plot) and the magnetic flux density norm on the ferromagnetic core.

- The AC/DC Module is used for simulating electric, magnetic, and electromagnetic fields in static and low-frequency applications
- Typical applications include capacitors, inductors, insulators, coils, motors, actuators, and sensors, with dedicated tools for extracting parameters such as resistance, capacitance, inductance, impedance, force, and torque

## COMSOL: AC/DC module
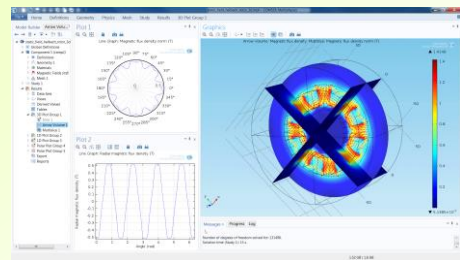


## Summary

- Many software packages are available for modeling of simple and complex devices, and transport processes
- Viable free options developed within academic environment
- Commercial packages are available for evaluation either in limited capacity, or for a limited time

## References

- A manual for AMPS-1D, The Center for Nanotechnology Education and Utilization, The Pennsylvania State University
- Y. Liu, Y. Sun, and A. Rockett, "A new simulation software of solar cells-- wxAMPS", Solar Energy Materials and Solar Cells, 2012
- M. Burgelman, P. Nollet, S. Degrave, Thin Solid Films 361 (2000) 527
- OrCAD Capture user manual, PSpice user manual
- An MCNP Primer, J. K. Shultis, R. E. Faw, Dept. of Mech. and Nuc. Engineering, Kansas State Univ., 2004-20011
- H.G. Hughes, "Features of MCNP6 Relevant to Medical Radiation Physics", presentation at RPSD-2012, Nara, Japan, LA-UR-12-24401 (2012)
- Introduction to COMSOL Multiphysics, www.comsol.com