SIMION™ Version 8

The Industry Standard in 3D Ion and Electron Optics Simulations

www.simion.com

Scientific Instrument Services, Inc.

1027 Old York Rd, Ringoes, NJ 08551

Phone: (908) 788-5550   Fax: (908) 806-6631

Scientific Instument
Services, Inc™

INL
Idaho National Laboratory

SIMION 8.0

S IMION 8.0 is a software package used primarily to calculate electric fields, when given a configuration of electrodes with voltages, and calculate trajectories of charged particles in those fields, when given particle initial conditions, including optional RF, magnetic field, and collisional effects. In this, SIMION provides extensive supporting functionality in defining your system geometry and conditions, recording and visualizing results, and extending the simulation capabilities with user programming. It is an affordable but versatile platform, widely used for over 25 years to simulate lens, mass spec, and other types of particle optics systems.

Typical usage of SIMION is illustrated below for a simple three-element Einzel lens. The geometry consisting of three ring electrodes with given voltages is defined (left), and the fields and particle trajectories are calculated and displayed (center and right).
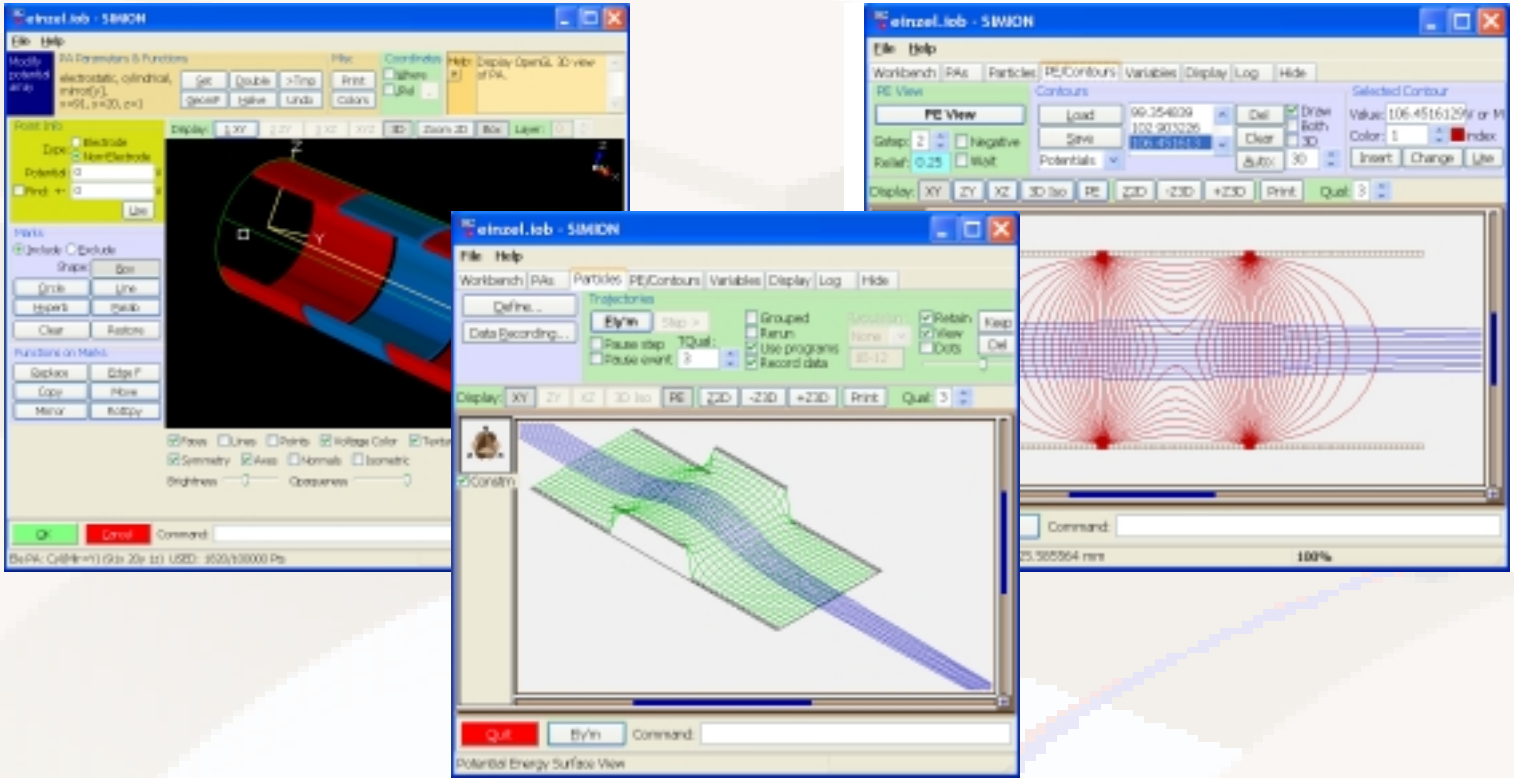
The main capabilities of SIMION are summarized on the following pages.

Electrostatic field solving: SIMION solves fields in 2D and 3D arrays of up to near 200 million points (2GB), with optimizations for systems with symmetry and mirroring, according to the finite difference method with much optimized linear-time solving. Small arrays solve in under a minute; very large arrays may take roughly an hour depending on conditions. A "workbench" strategy allows you to position, size, and orient up to 200 array instances (3D images) of different grid densities and symmetries to permit the simulation of much larger systems that don't easily fit into a single array. Some magnetic field solving capabilities are also available (see following page).

Particle trajectory solving: Particle trajectories are calculated given the previously calculated or defined fields. The method is Runge-Kutta with relativistic corrections and variable-length dynamically adjusting and controllable time steps. Particle mass, charge, and other parameters can be defined individually or according to some pattern or distribution. User programming can modify the system during particle flight to inject novel effects (such ion-gas scattering). Particle tracing is fast – millions of particles can be handled—and they display in real-time. Basic charge repulsion effects can help estimate the onset of space-charge (though for more advanced and numerically accurate space-charge and space-charge limited cathode emission calculations, we recommend our CPO software).

Viewing of the system is highly interactive, allowing adjustment of parameters and viewing of the system even during particle flight (trajectory calculation). SIMION supports cutting away volumes to see trajectories inside, zooming, viewing potential energy surfaces, contour lines, and trajectories, and reflying particles as dots for movie effects. Nice OpenGL viewing of arrays (above-left) is also available.
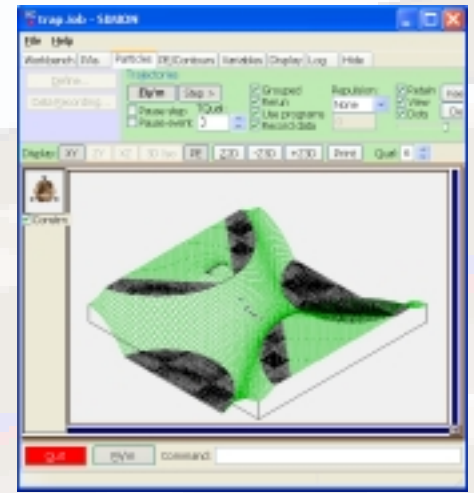
Applications

S IMION is suitable for a wide variety of systems: from ion flight through simple electrostatic and magnetic lenses to particle guns to highly complex instruments, including time-of-flight, hemispherical analyzers, ion traps, quadrupoles, ICR cells, and other MS, ion source and detector optics.
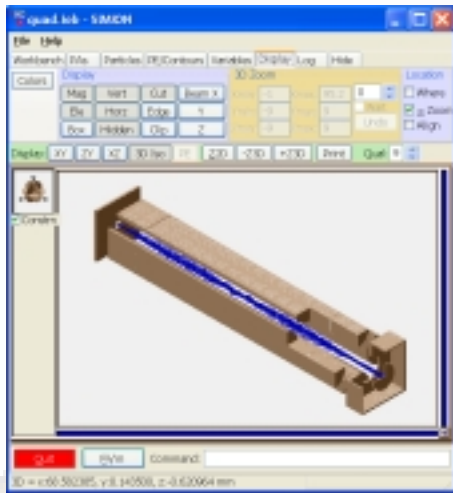

**RF Quad Mass Filter**
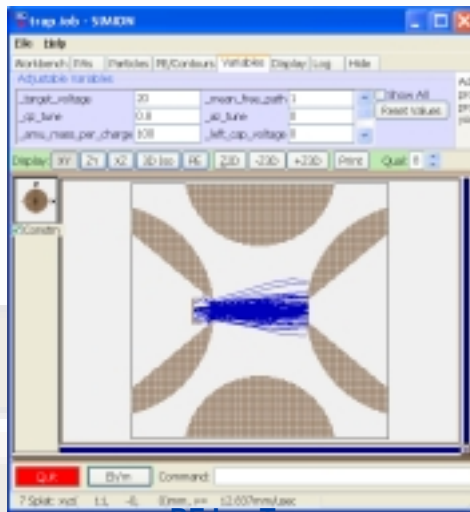
RF Ion Trap

RF Ion Trap (Potential Energy Display)

Time-dependent or RF (low frequency) voltages: Electrode voltages may be controlled in a general way during particle flight via simple user programs – e.g. to step or oscillate electrode voltages in some manner. Quadrupole mass filter, multipole, and ion trap simulations **(above)** in the megahertz range are regularly performed. SIMION applies the quasistatic approximation with superposition, which gives fast calculations (but assumes the absence of induced magnetic field or radiation effects as would occur in "high frequency" systems having the wavelength below the length of your system).
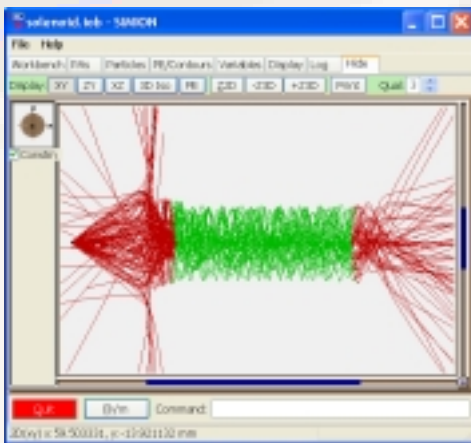

**Ion Confinement in Air Solenoid**
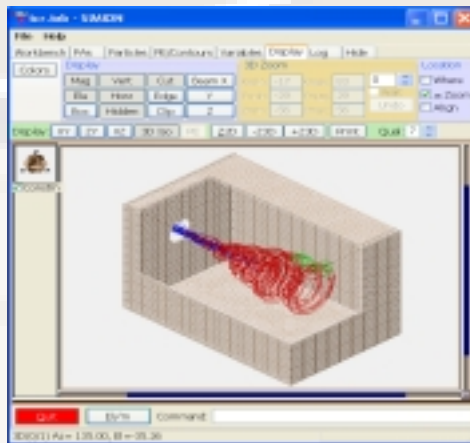
ICR Cell

Magnetic fields: SIMION will solve magnetic fields in the restricted case involving scalar magnetic potential (no permeability) via the same Laplace methods as the electrostatic case, and it will solve magnetic fields from wires/solenoids (left) by Biot-Savart calculations. Also, an arbitrary (vector) magnetic field can be imported from an external program or defined analytically, optionally superimposed on an electrostatic field (e.g. penning trap or ICR cell – right) for the purpose of particle flying.

Ion-neutral collisions: SIMION can handle the effects of particles colliding against a background gas, such as for the buffer gas of the ion trap (top), the background gas in an RF ion-funnel (right), or in ion mobility. Multiple collision models are included: Stokes' law, hard-sphere, and a model optimized for high pressure "atmospheric" conditions. The particles will diffuse and randomly scatter away from their normal trajectories.
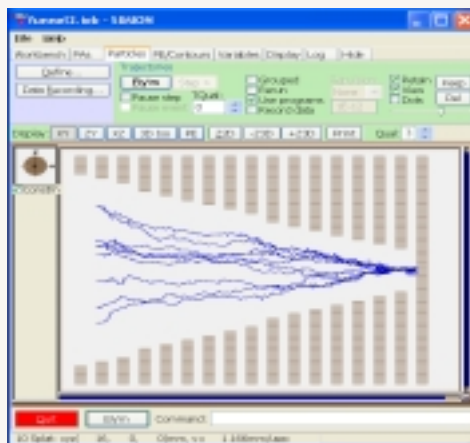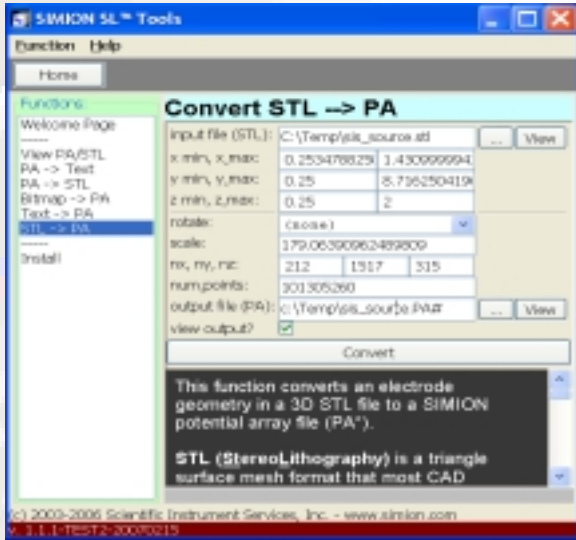

**RF Ion Funnel**
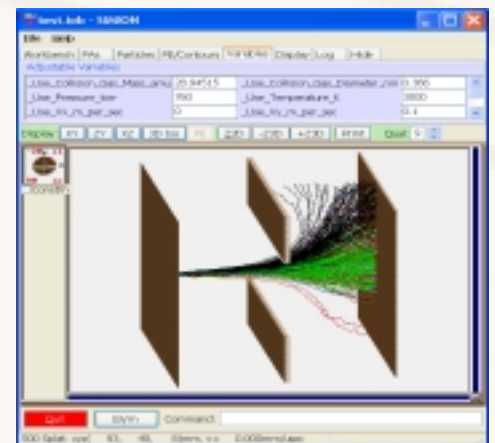
Atmospheric Pressure Example

Simulation Setup

SIMION includes an assortment of features for setting up your simulation.

Geometry definition: A system geometry can be defined by whichever method is most convenient for you: an interactive **3D paint-like program** (called "Modify"), **CAD import from STL** format (supported by most CAD packages), a **solid geometry defined mathematically via a text file** ("GEM files"), and programmatic manipulation of arrays from such languages as Perl, Python, and C++ ("SL Libraries"). An application called **Virtual Device**, available separately, provides a GUI for creating GEM files too.


Complex CAD Model imported from STL file (left) to a SIMION array (right).
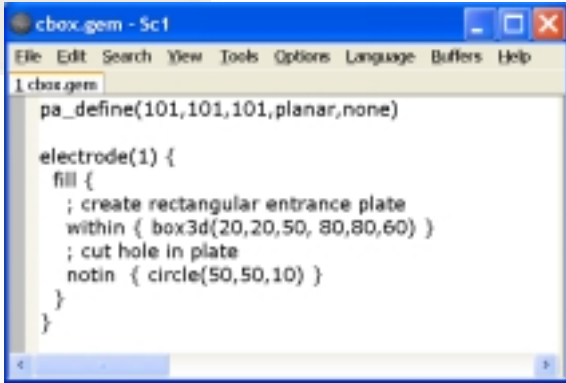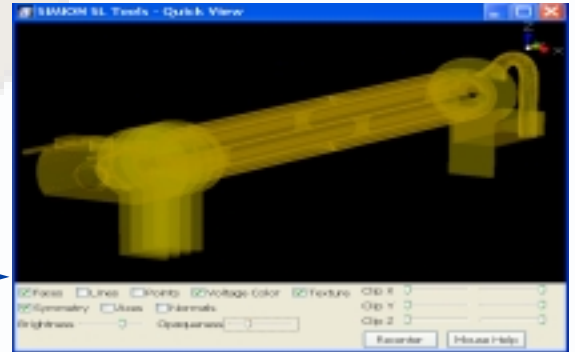
Geometry (GEM) definition file example (left) and result (right).
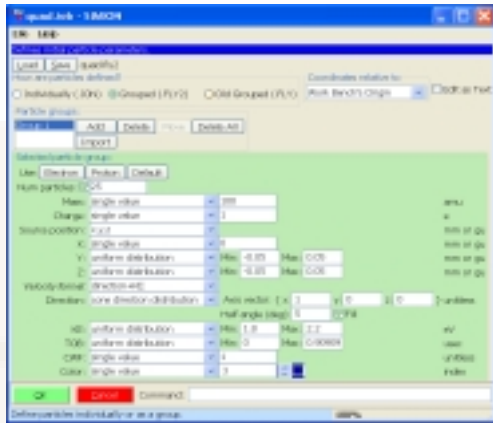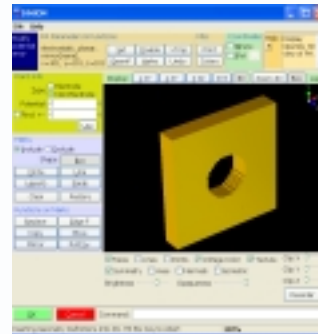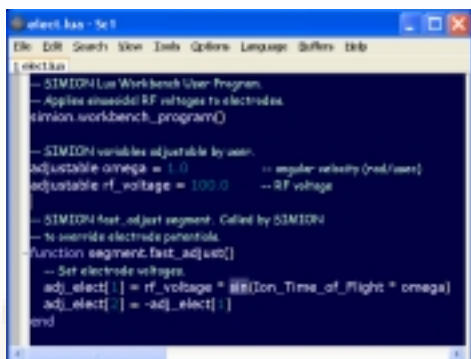

Particle initial conditions can be defined in various ways. A much extended "FLY2" format in SIMION 8 allows quick definition of many types of particles random distributions and sequences. Particles may also be exhaustively enumerated (optionally imported from a text file).
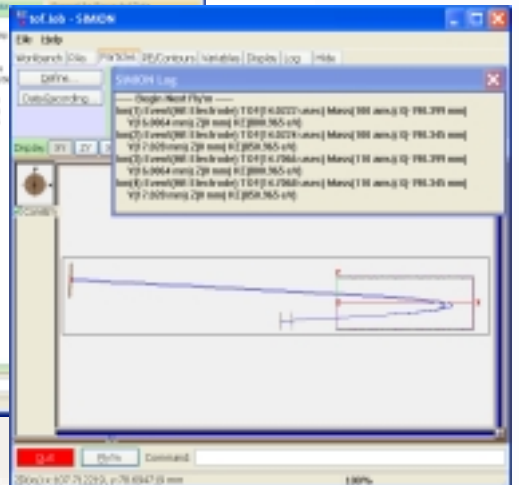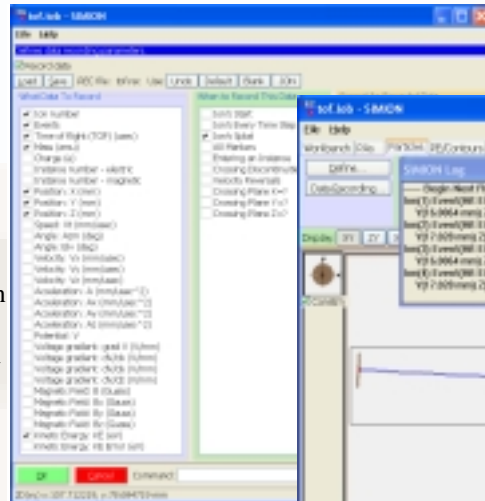
Data recording: The simulation parameters you are interested in (e.g. ion position, velocity, KE, and voltage) can be recorded at various stages in particle flight (e.g. when hitting an electrode and crossing a plane). Data can be recording to the screen (right) or to delimited text file for subsequent analysis of fields and trajectories. Analysis can be done via SIMION user programming (see next page), in a program or language of your choice like Excel (see next page), or in the Virtual Device program (available separately with various convenience plotting and analysis functions).

Analysis and Customization

SIMION has a number of capabilities for collecting data.

Programming in Lua

User programming allows the simulation to be extended in many novel ways. During ion flight, you may control electrode voltages (example at left), define or modify fields, scatter or deflect ions (e.g. ion-gas collision models), tune (optimize) lens voltages, compute results, export data to programs like Excel via COM or command-line interfaces, and do many other things. The **Lua scripting language** (new in version 8) is directly embedded in SIMION, and Lua may also call C/C++ or COM routines. Programming may also be used to operate SIMION in **batch mode**, such as for geometry optimization or to read/manipulate potential array files.

**In the example at right, trajectories are calculated while phase space data is interactively plotted in Excel via the Lua COM interface**
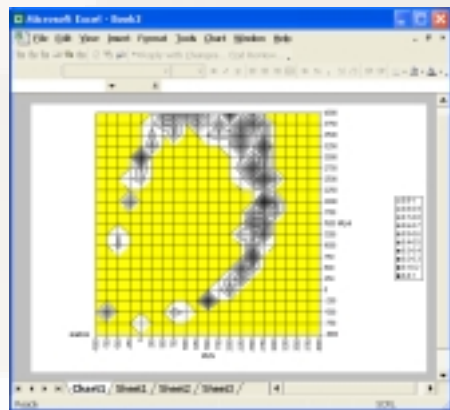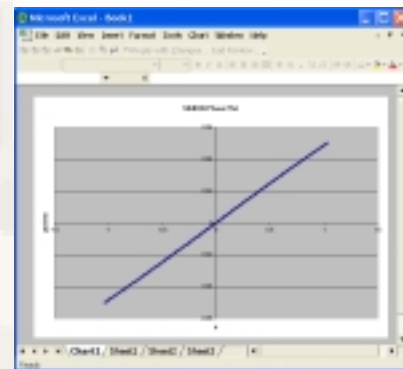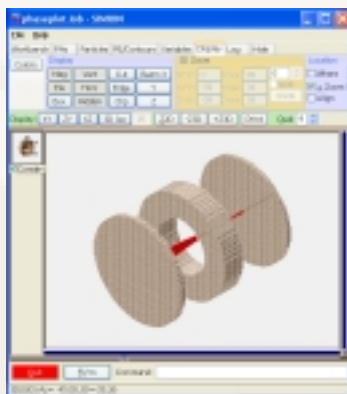
SIMION can optimize voltages and geometry with simplex optimizer and batch mode capabilities. At left is a SIMION generated surface plot of beam size as a function of two lens voltages. At right is one of the many user programming examples (scattering at surface).

Surface Plot in Excel
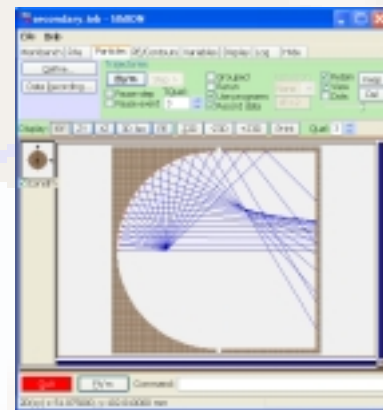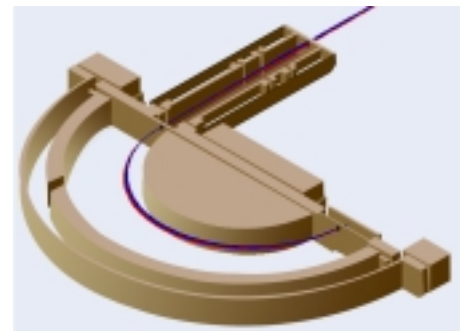
Scattering Effects at Surface

Contents

- • **Package contents:** a 450-page printed manual, installation CD with software license key number (for receiving software updates), and quick start notes. The installation CD installs the software, examples, and additional documentation.

- • **Documentation:** SIMION comes with a 450-page printed manual. Additional documentation and course notes are available electronically, in the examples, or on the simion.com web site. See the www.simion.com web site for the user group, software updates, latest SIMION tips, articles, and links to some of the hundreds of scholarly papers that use SIMION.

- • **Updates:** Free upgrades to 8.0.x versions released within a year of 8.0.0 are provided as free downloads from simion.com.

- • **Support:** Limited free support via email and phone is included, and there is also an open message board.

- • **Supported systems:** Formally tested on Windows Vista, XP, 2003, 2000, and NT, as well as Wine/Linux (Intel Macs with CrossOver also reported). Latest system compatibility information is on www.simion.com.

Major Changes Between SIMION 7 and SIMION 8

This list is provided for the convenience of SIMION 7 users. For a more complete and up-to-date list of changes, see www.simion.com.

- **Major revamp of user interface:** Includes native GUI controls and file manager (more standard), OpenGL viewing of PA files, reduced screen flicker (double-buffering), and clear labeling and placement of functionality to reduce learning curve.

- **Enhanced user programming:** The **Lua programming (scripting) language** is now embedded into SIMION and supplants PRG (though PRG, and SL which compiles down to PRG, is still supported for compatibility). **Batch mode operation** including a command-line and Lua APIs allows SIMION to be controlled by an external program (e.g. GEM --> PA, refine, fast adjust, and fly). One batch mode example included performs **geometry optimization.** Programming libraries (SL Libraries from the SL Toolkit and new Lua libraries) are included.

- **CAD Import:** CAD import (STL format) and other import/export functions (from the SL Toolkit) are included. Note: SIMION 8 replaces the SL Toolkit, which will no longer be sold separately.

- **New particle definition format:** Supports new "FLY2" particle definition format, which simplifies the definition of particle sequences and randomized distributions. (Original FLY is still supported for backward compatibility though.)

- **Expanded limits:**
  - **Max PA size** slightly increased from 50 million (in 7.0) to almost 200 million (if sufficient RAM available ~2GB).
  - **Maximum fast scalable and fast adjustable electrodes** increased from 31 to 128.
  - **Max number of particles** increased from 500 thousand (in 7.0) to about 10 million (if sufficient RAM available).

- **Improved performance:** Initial measurements show refine and fly times reduced by ~20-40% from 7.0, largely due to compiler and display optimizations.

- **New/updated examples:** PRG programs have been rewritten in Lua, and documentation has been expanded. A number of new examples have been added such as geometry optimization, phase plotting in Excel (via Lua COM), HS1 ion-gas collision model, SDS "atmospheric pressure" collision model, beam emittance calculation, ion funnel, IMS, simplex optimization (8.0.3), air core solenoid magnetic field, field import and interpolation from text file, and hemispheric deflection analyzer shown below (with voltage optimization and Excel plotting).

- **Excel and COM control** via Lua – demonstrated in new "Excel" examples – provides enhanced plotting and data analysis capabilities.

- **Magnetic fields from wire currents** (e.g air core solenoids) by Biot-Savart calculations − demonstrated in new "solenoid" example.

- **Optimization of voltages and geometry** with simplex optimizer and batch mode capabilities – demonstrated in new HDA and geometry optimization examples.

- **New ion-gas collision models** – low pressure hard-sphere (HS1) and high pressure (SDS) models.

- **Multiple sets of fast scalable electrodes** (8.0.3) − Reduces number of fast adjustable electrodes in the new "ion funnel" example.

- **Free 8.0.x software updates** for one year after the initial 8.0.0 release.

- **Updated 450 page manual**

Part No.	Description
SIMION8	SIMION 8.0 (commercial pricing)
SIMION8A	SIMION 8.0 (US academic/government)
SIMION8U(SIMION8U2)	SIMION 8.0 (upgrade from 7 or SL)
SIMION8LK	SIMION 8.0 (academic site license – 30 seats)