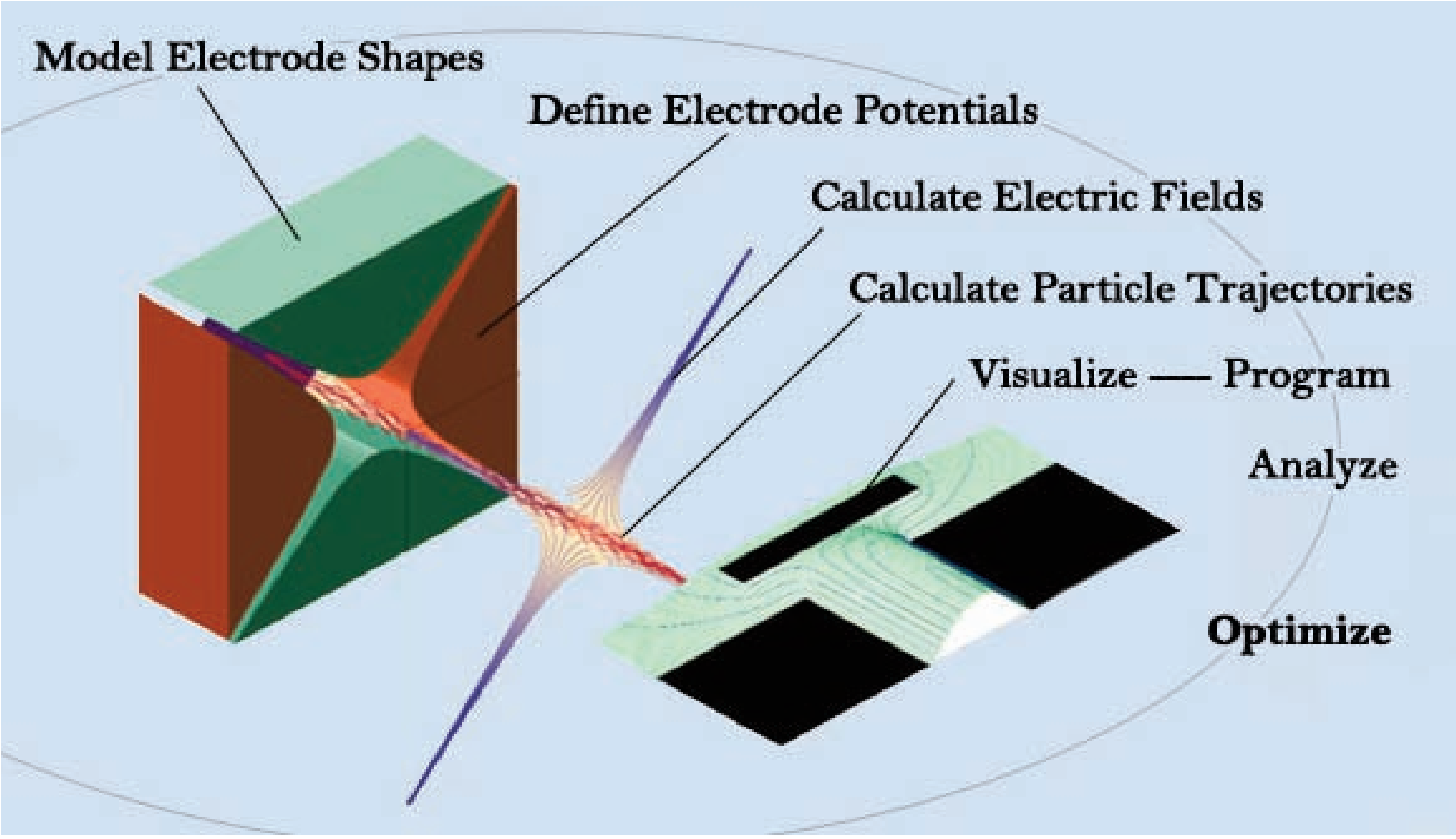
# SIMION™ Version 8.1

***The Industry Standard in 3D Ion and Electron Optics Simulations***




**www.simion.com**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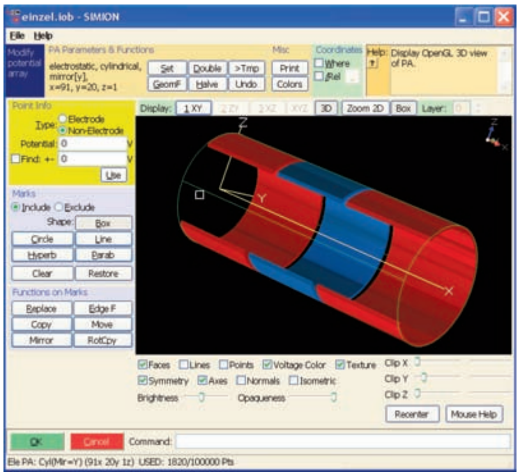
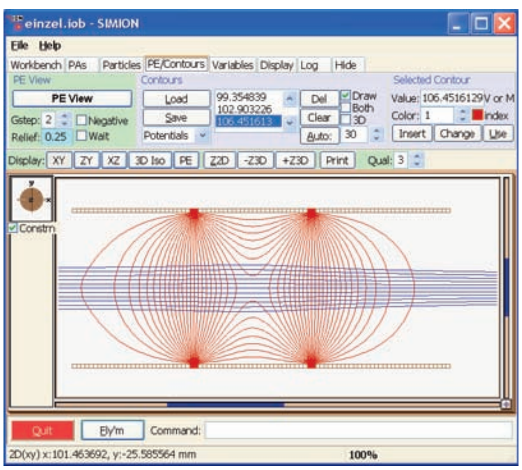
# SIMION 8.1

SIMION 8.1 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 are supported. 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 35 years to simulate lens, mass spec, and other types of particle optics systems.

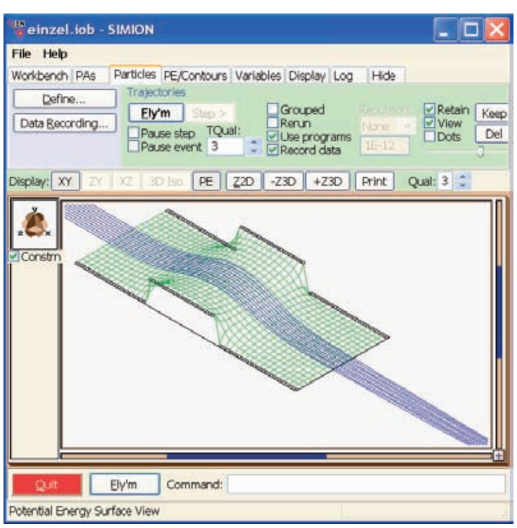
Typical usage of SIMION is illustrated below for a simple three-element Einzel lens. The geometry consisting of three ring electrodes with given voltages is defined (top), and the fields and particle trajectories are calculated and displayed.




**Electrostatic field solving:** SIMION solves fields in 2D and 3D arrays of up to near billions of points, 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 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).



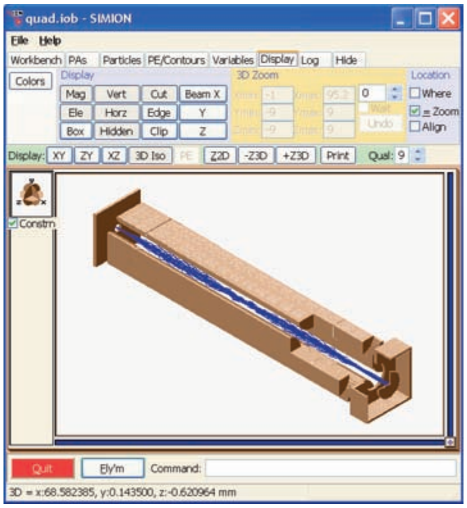

**Particle trajectory solving:** Particle trajectories are calculated given the previously calculated or defined fields. The method is Runge-Kutta with relativistic corrections and variable-length dynamically adjusting and controllable time steps. Particle mass, charge, and other parameters can be defined 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, including a poisson solver can help estimate the onset of space-charge.



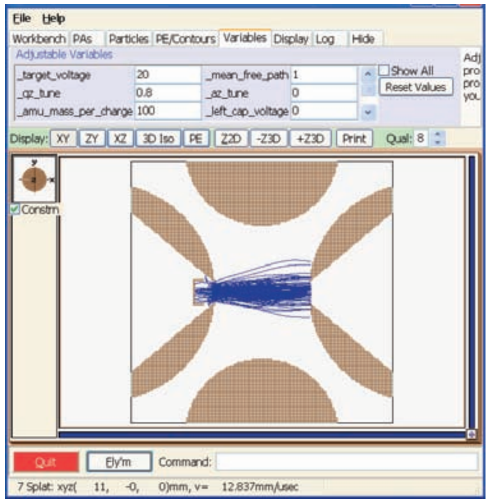

**Viewing of the system is highly interactive**, allowing adjustment of parameters and viewing of the system even during particle flight (trajectory calculation). SIMION supports cutting away volumes to see trajectories inside, zooming, viewing potential energy surfaces, contour lines, and trajectories,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

# Applications

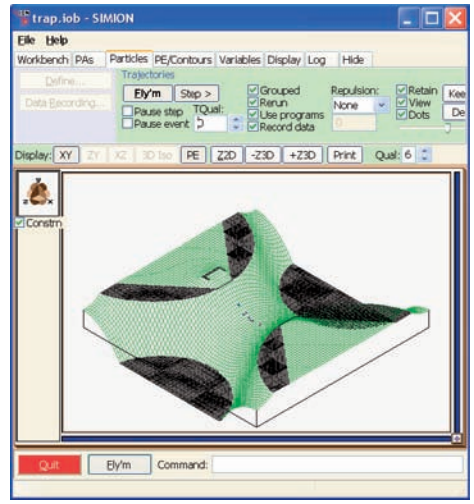
SIMION is suitable for a wide variety of systems: from ion flight through simple electrostatic and magnetic lenses to particle guns to highly complex instruments, including time-of-flight, hemispherical analyzers, ion traps, quadrupoles, ICR cells, and other MS, ion source and detector optics.




RF Quad Mass Filter

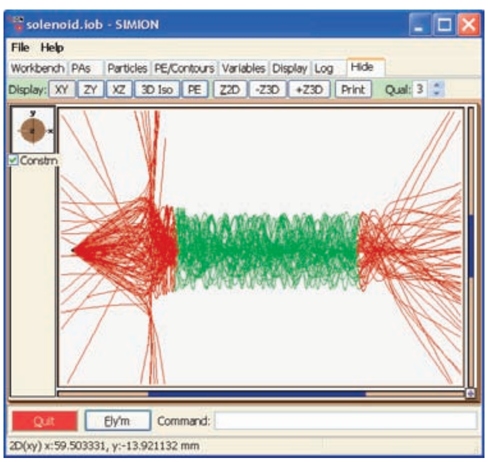


RF Ion Trap

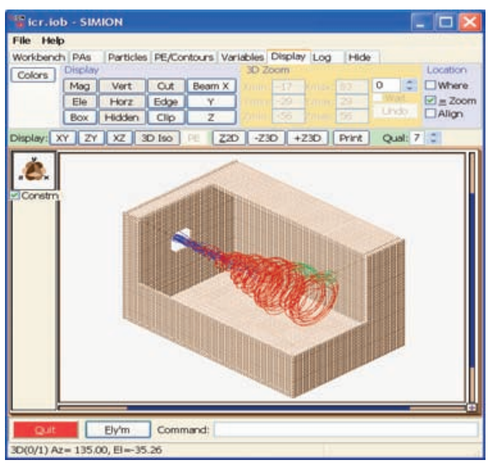



RF Ion Trap (Potential Energy Display)

**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 (assuming 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).



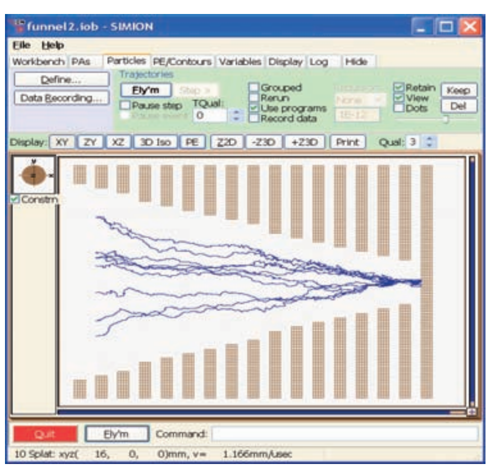

Ion Confinement in Air Solenoid



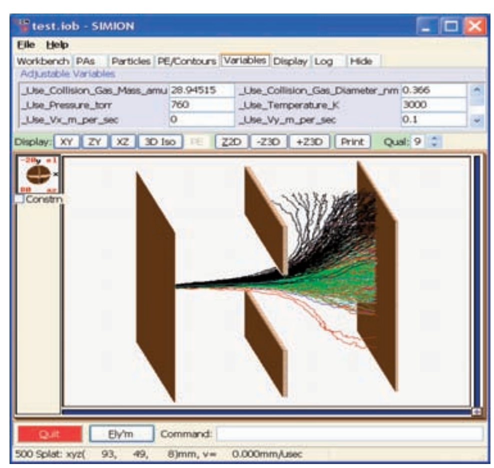

ICR Cell

**Magnetic fields:** SIMION will import magnetic fields, define them analytically or solve them in restricted cases (e.g. Biot-Savart wire currents - left), 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 mobility model optimized for high pressure "atmospheric" conditions. The particles will diffuse and randomly scatter away from their normal trajectories.



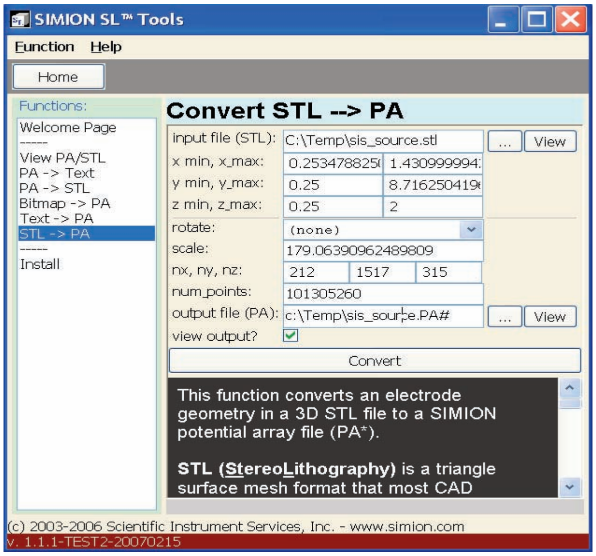

RF Ion Funnel



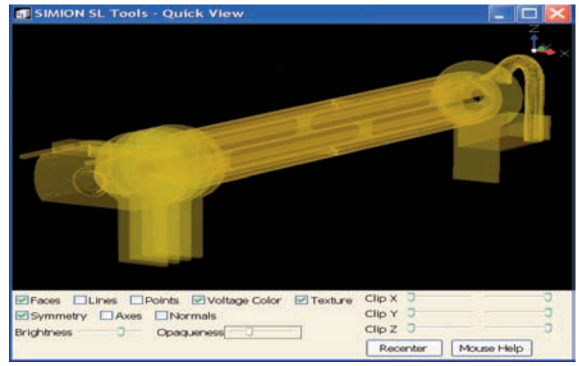

Atmospheric Pressure Example

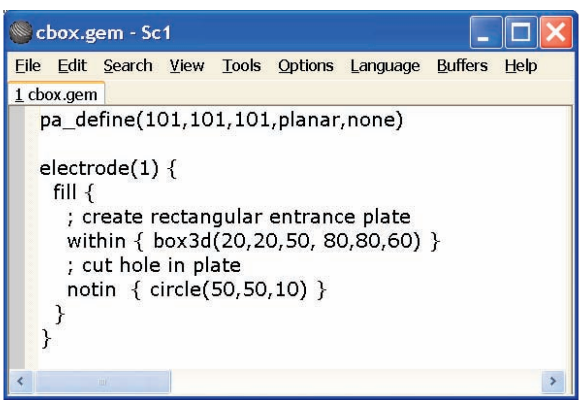
# Define Your Simulation

**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 Lua, Perl, Python, and C++.

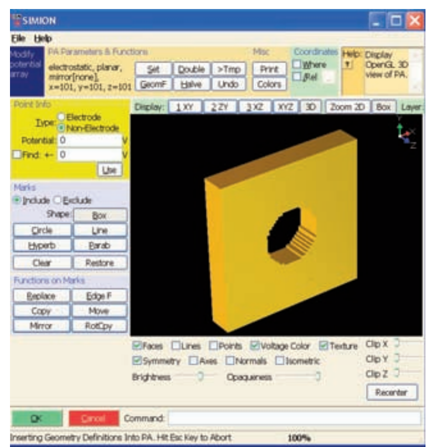


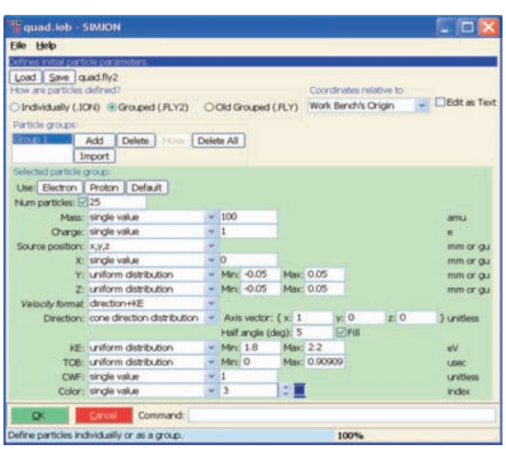

**Complex CAD Model imported from STL file (left) to a SIMION array (right).**




**Geometry (GEM) definition file example (left) and result (right).**



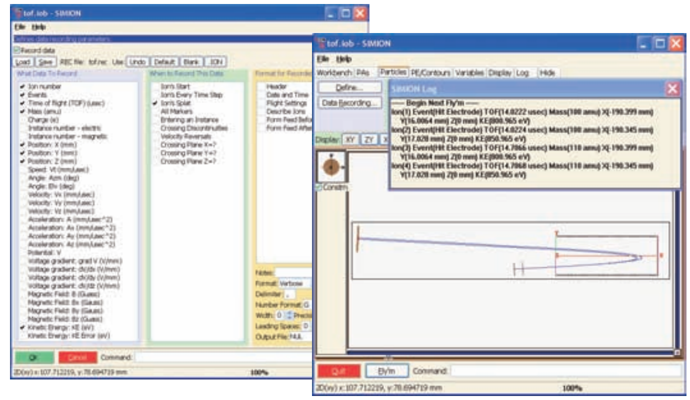



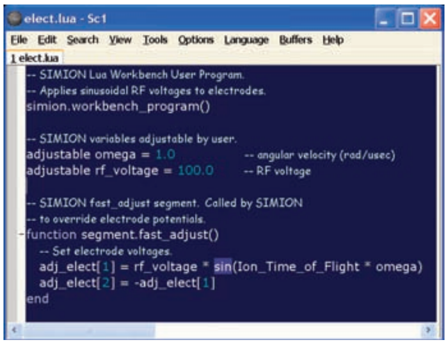

**Particle initial conditions** can be defined in various ways. The "FLY2" format in SIMION allows quick definition of many types of particles random distributions and sequences. Particles may also be exhaustively enumerated (optionally imported from a text file).

# Analysis and Programming

SIMION has a number of capabilities for collecting data.

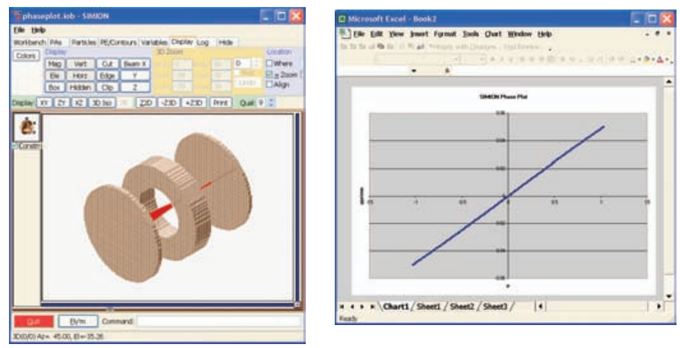
**Data recording:** The simulation parameters you are interested in (e.g. ion position, velocity, KE, and voltage) can be recorded at various stages in particle flight (e.g. when hitting an electrode and crossing a plane). Data can be recording to the screen or to delimited text file for subsequent analysis of fields and trajectories (right). Analysis can be done via SIMION user programming, in a program or language of your choice like Excel, and MATLAB®.



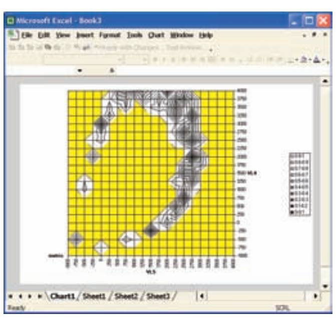



**Programming in Lua**

**User programming** allows the simulation to be extended in many novel ways. During ion flight, you may control electrode voltages (example at right), 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** 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.

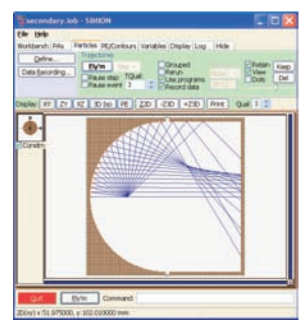


**In the example above, trajectories are calculated while phase space data is interactively plotted in Excel via the Lua COM interface**



**Surface Plot in Excel**

**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).**



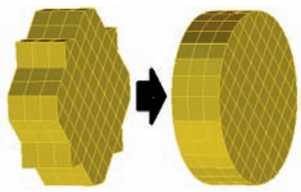
**Scattering Effects at Surface**

# Contents

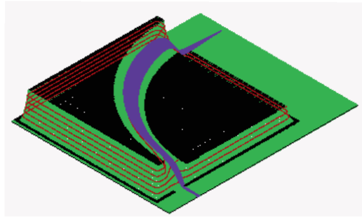
- **Package contents:** a 450-page printed manual, installation CD with software license key number (for receiving software updates), and quick start notes. The installation CD installs the software, examples, and additional documentation.
- **Documentation:** SIMION comes with a 450-page printed manual. 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 updates to 8.1.x versions of 8.1 are provided as free downloads from simion.com.
- **Support:** Free basic support via email, phone, and forum
- **Supported systems:** Formally tested on Windows 10/8.1/8/Vista/XP, as well as Wine/Linux (and Crossover/Mac). Latest system compatibility information is on www.simion.com.

# Features in SIMION 8.1 (and 8.2EA/beta)

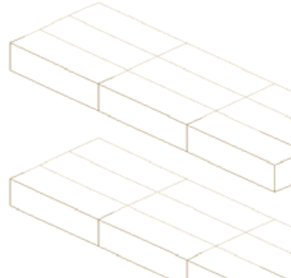
## More Accurate



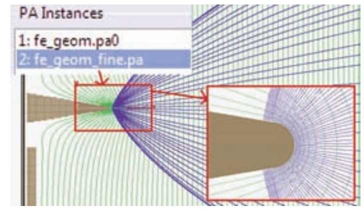
Improved curved surface handling (“surface enhancement”) gives order of magnitude field accuracy improvement



Large 64-bit array sizes up to 20 billion points / 190 GB

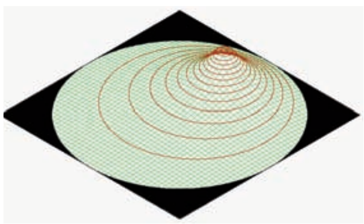


Oblong, non-square grid cells.



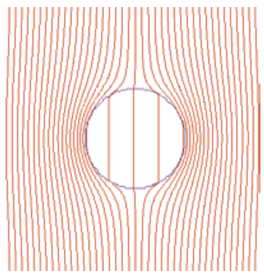

Nested refining techniques

## More Versatile



Poisson solver (Refine), fully programmable

Example: charged sphere in grounded tube

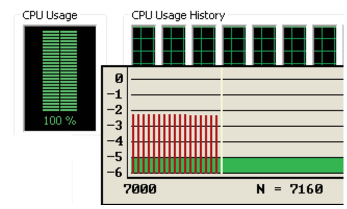


Dielectric materials (Refine)

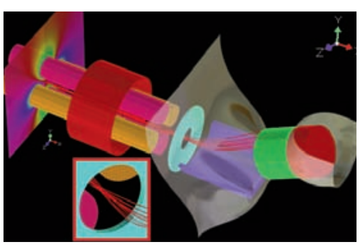
Example: dielectric sphere in E-field

Some permeability and magnetic vector potential features (Refine) [8.2EA]

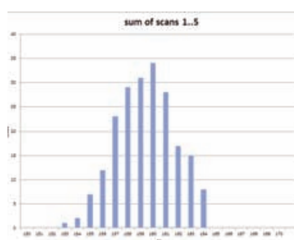
### Speed and Compatibility



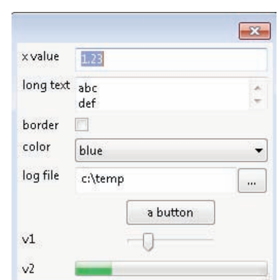

Multicore Refines (8.1)
Multicore Fly’m (8.2EA)
Native Linux batch mode binary (8.2EA)



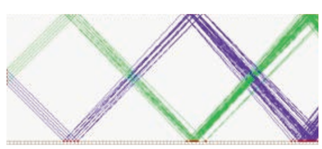
High quality 3D (OpenGL) graphics on View screen [8.2EA]
Programmable plotting capabilities for B-fields, gas flow, and wire coils.




Integration with Lua/C, Excel, gnuplot, Origin, VirtualDevice , MATLAB® (8.2EA), various magnetic/gas solvens like Fluent and Superfish (8.2EA) and other programs.

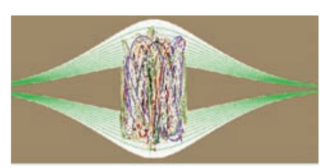



New GUI dialog library (8.2EA)



New programming API’s: new segments for run automation (initialize_run, terminate_run, flym) [8.1.1], updating and refining geometries within the View screen, manipulating the model from Lua, creation of secondary particles, and more.


Supplemental Documentation expanded



More examples and documentation