

## FEATURES

### NEW - Agilent Flip Top Inlet Sealing System .....2

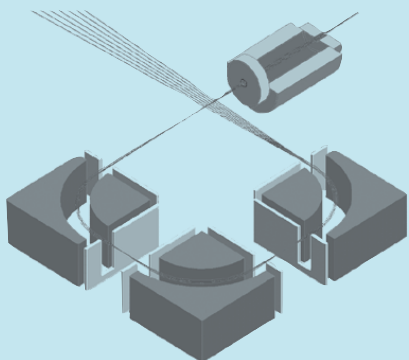
A device designed to allow the user of Agilent's GC's to safely and reliably change an inlet liner in as little as 30 seconds without any tools in a consistent leak-free manner.

### NEW - SIMION SL Toolkit . . .10

A new utility pack for expanding the capabilities of the SIMION 7.0 Ion Optics Simulator.

### SIMION Web Site and Discussion Group

[www.simion.com](http://www.simion.com)



SIS has established a new SIMION Web site with links to information related to SIMION. We have also set and will be monitoring a new SIMION users group. See the back cover of this newsletter for additional details.

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For Mass Spectrometry and Chromatography

## NEW! SIMION SL

SIS has developed a new accessory package to expand the capabilities of SIMION. One of the most frequent requests from SIMION users over the years has been the ability to import drawings from other CAD or drawing packages into SIMION. SIS undertook this challenge and has written custom software to enable structures designed in other packages to be converted into files that can be used in SIMION. This is only one of the many new features included in this new software accessory package available exclusively from SIS. For additional details see the article on SIMION SL in this newsletter or for more information visit the SIMION web site at <http://www.simion.com>

## The Tradition Continues at ASMS

SIS will once again be sponsoring the SIS "Make Your Own Ice Cream Sundae" Hospitality Suite at the ASMS meeting in Nashville, TN. Our Hospitality Suite will be open on Monday and Tuesday evenings (5/24/04 and 5/25/04) from 8:00 till 10:00 p.m. DeTech will also be sharing our hospitality suite and will once again be distributing their 2004 ASMS Souvenir Cup - but come early because they go quickly. Stop by our hospitality suite to meet the staff from SIS and DeTech to discuss any technical issues you might have and to help us serve you better.

During the week we will also be having some one-on-one demos and training on SIMION and SIMION SL in our hospitality suite. If you are interested in learning more about these products or would like some instruction on the use of SIMION, please let us know to make an appointment.

Join S.I.S.  
for a Sundae



# Agilent Flip Top Inlet Sealing System

**NEW**

for the Agilent 6890, 6850 & 5890 GC's

*The faster, smarter way to change inlet liners on Agilent GC's*

## Features

- Cuts liner replacement time to as little as 30 seconds
- No more frustrating searches for special wrenches or tools
- Improved inlet ergonomics - No more handling of heated parts, no more burns or scrapes
- Decreased downtime = increased productivity
- Minimizes exposure to ambient air extending column life
- Installs easily in 15 minutes (by the customer)

Agilent's new Flip Top Inlet Sealing System is a device designed to allow the user of Agilent's GC's to safely and reliably change an inlet liner in as little as 30 seconds in a consistent leak-free manner without any tools. No longer will your customers have to contend with frustrating searches for special wrenches or burn their fingers on hot inlets.

The Flip Top has a levered arm that attaches to any 6890/6850/5890 insert weldment and locks to the injection port using an adapter ring screwed onto the inlet. Once installed, the user simply lifts the arm of the Flip Top which releases the insert weldment from the injection port, and allows instant access to the liner. The process is simply reversed to re-seal the weldment to the port.



Simply lift the arm of the Flip Top, which releases the insert weldment from the injection port and allows instant access to the liner.



Part No.	Description
5188-2717	Flip Top Inlet Sealing System
5188-2741	Inlet Liner O-rings for Flip top 10/pk

## Terms and Conditions

Scientific Instrument Services (S.I.S.) continues to supply "The Mass Spec Source" newsletter as a service to our customers. Printed four times a year, it includes articles and notes on new products and procedures of interest to mass spec and GC users. Papers from all fields of scientific inquiry in which mass spectrometry and gas chromatography can play a role will be considered and subject to review. However, S.I.S. reserves the right to reject any article that is in direct competition with S.I.S. products.

## Articles and Application Notes

Editorials and reviews on new instrumentation and techniques for GC/MS will be considered for publication. These articles may be any length and our Graphics Department will aid you in any way you may need.

## Mass Spec Tips

Any new ideas or tips that could benefit other mass spectroscopists can be submitted for inclusion in this section.

## For More Information

Anyone interested in writing in any of the areas above should contact the editor of the Mass Spec Source, at (908) 788-5550. We are always trying to improve this newsletter, if you have any suggestions please give us a call. Thanks for your continued support.

## Warranty

S.I.S. does not warranty that the items described herein are usable or fit for a particular purpose. Our company makes no representation as to condition or character of the merchandise. S.I.S. will not be responsible for consequential or special damages.

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## Introducing the SL Toolkit for SIMION A New Utility Pack for Expanding the Capabilities of the SIMION 7.0 Ion Optics Simulator

By David Manura, Scientific Instrument Services, Inc., 1027 Old York Road, Ringoes, NJ 08551

**S**IMION has proven quite versatile over the years in its widespread use in both industry and academia in modeling the ion optics of mass spec components and various electrostatic and magnetic systems. However, as customers have provided feedback, the capabilities of SIMION 7.0 are not without their limitations:

- (1) Drawing electrode geometries can be cumbersome, especially if you need to redraw your complicated CAD models in SIMION,
- (2) The "PRG" user programming language is relatively low-level and takes some extra effort to understand.
- (3) Some data import/export features are missing or require extra effort, such as importing/exporting a refined potential array to/from a text file.

SIS has addressed these and other limitations by developing the "SIMION SL Toolkit" (Simple SIMION Language and Toolkit), which is a collection of utilities and files providing added value to your SIMION system.

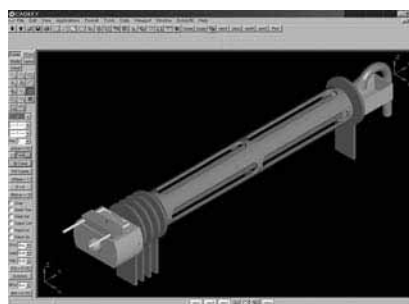
The SIMION SL Toolkit contains these components:

- Potential Array (PA) Tools
  - o Convert 3D CAD (STL) files from your favorite CAD package to 3D SIMION PA files.
  - o Convert 2D bitmap image files to 2D SIMION PA files
  - o Extract potential and potential gradient (i.e. field) maps as ASCII text files from refined PA files.
  - o Convert PA files to STL files.
  - o Quickly view PA and STL files from Windows Explorer (OpenGL viewer)
  - o C++/Perl/Python libraries for programmatically manipulating SIMION potential array files.
- SL Compiler
  - o Write SIMION user programs in a high-level SL language rather than in PRG code.
- Miscellaneous Utilities: Text editor plug-ins (syntax highlighting) and other enhancements.

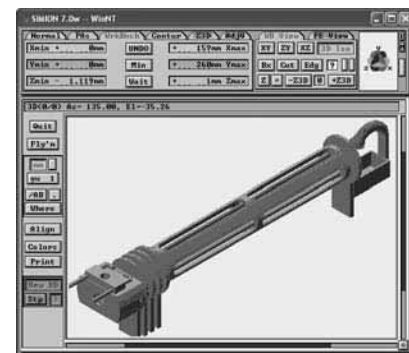
This list will continue to expand, and as it expands SL customers can download updates from our web site ([www.simion.com](http://www.simion.com)). In fact, a number of the components, including the compiler and C++/Perl/Python libraries, come with full source code included. We appreciate feedback and suggestions on the toolkit.

### CAD Import/Export

**T**he first major feature of SL is the ability to easily convert from a CAD model drawn in one of many CAD software programs available to a SIMION potential array (PA) file:



**Figure # 1** – CAD Drawing of a Source, Quadrupole Filter and Detector. (CADKEY solids)



**Figure # 2** – SIMION Potential Array File of the same Source, Quadrupole Filter and Detector transferred to SIMION using the new SIMION SL Toolkit.

Shown above, a source, quadrupole filter, and detector geometry was drawn in a CAD software package (CADKEY solids) and exported as an STL file, which is a format that CAD packages can export. The STL file was then loaded into one of the SL utilities named `patools.exe`, which converted the STL file to a SIMION PA file (shown in the above SIMION workbench).

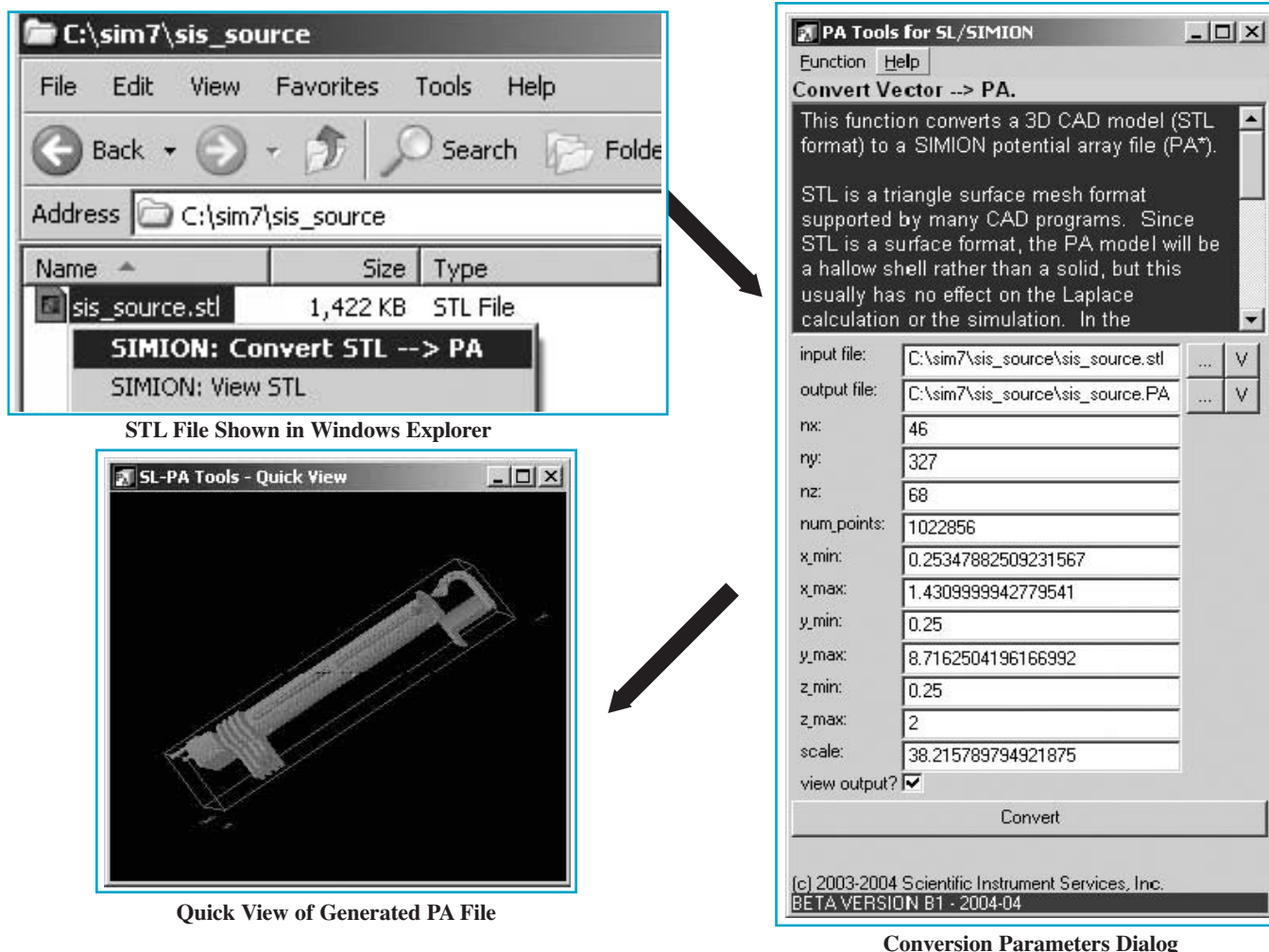
This new method of geometry definition augments the two methods built into SIMION 7.0: the GUI editor (the "Modify" function) and the geometry (GEM) files. The GUI editor is like a 3D paint program, which suffers largely in that the geometry can become distorted if you need to resize (resample) your model. The GEM file is an ASCII text file representing a vector format in which your solids are defined according to constructive solid geometry (CSG) operations, not unlike in most CAD programs. Although unaffected by resizing effects, the main downsides are that the GEM files lack some primitives needed for easily creating certain arbitrarily shaped surfaces, and the user may wish to create geometries in one's standard CAD software rather than recreate the GEM files by hand.

We now turn to two questions: How easy is the conversion process? Does this work with your particular CAD software?



## Ease of Use

At a minimum, the conversion process can take a few clicks, but you may want to make additional adjustments to the default scaling and electrode potentials. To convert an STL file, right click on the file in Windows Explorer and select "SIMION: Convert STL → PA." A dialog box will display providing various conversion parameters. You may accept the defaults and press "Convert." This creates the corresponding PA file, which will immediately display in a viewer that you can rotate with your mouse.



**Figure #3** - 3 Steps of File Conversion to SIMION

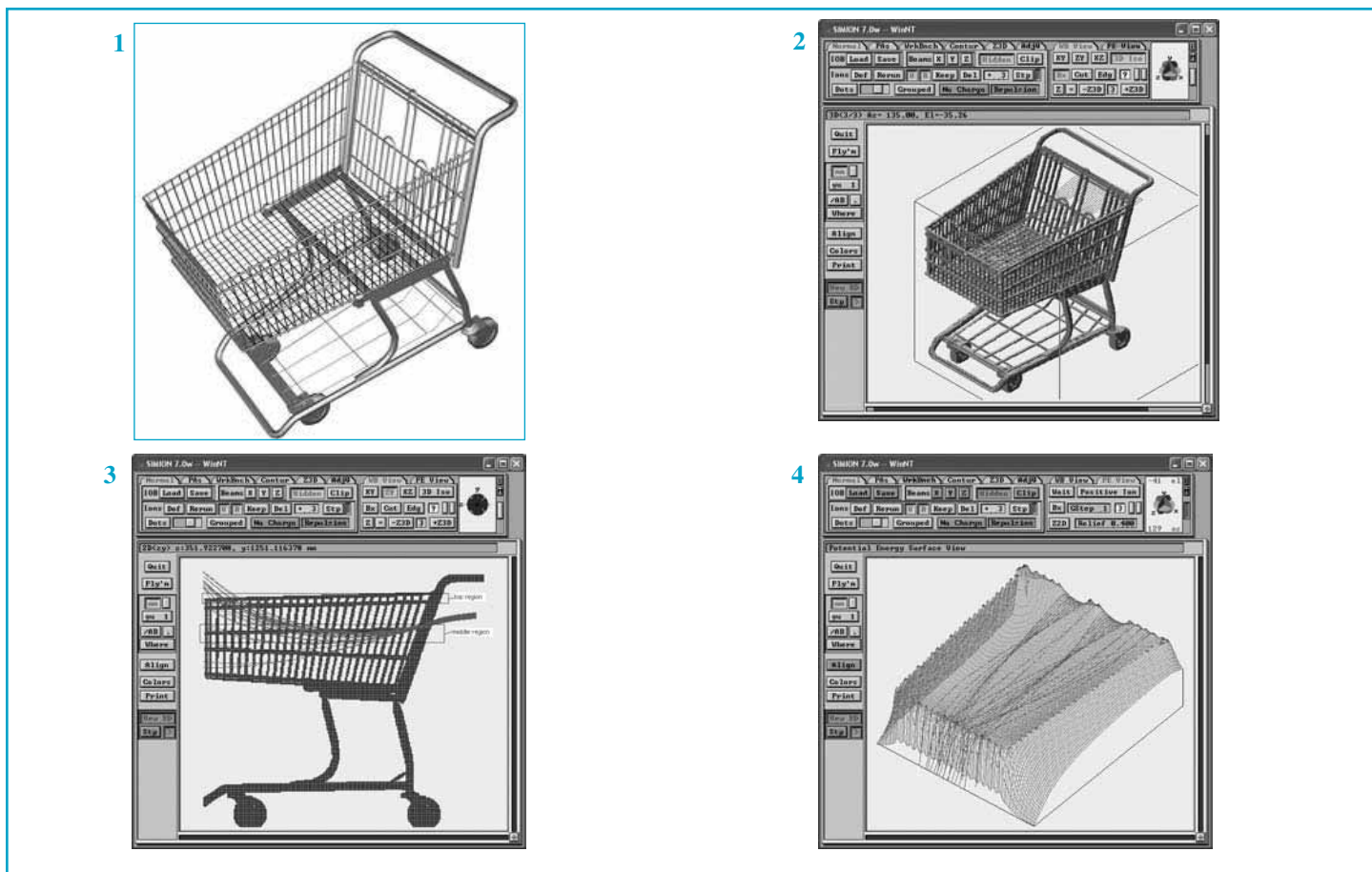
The parameters in the conversion dialog allow you to change the number of grid points in the potential array and the scaling of it. Readily accessible context sensitive help is provided for each parameter.

One caveat is that STL files do not contain layering or coloring information, so SIMION SL sets all solid points in the potential array to 1 V. Potentials can be easily changed subsequently, however, using the Modify function in SIMION. In particular, you can use the "Find" sub-function to search and replace the potential values of all electrodes points within some volume region of your model. This was done for the quadrupole.

## Supported Cad Packages

Most CAD software can export the STL format. STL is a fairly low common-denominator format representing the surface of your solid as a triangular mesh. Although basic, such a format is largely sufficient for the purpose of rasterization into the SIMION PA format, so that is why we choose it. STL is, however, a surface format not a solids format, so your models actually will be hollow shells when imported into SIMION. Luckily, the interior of your electrodes (or lack thereof) has no effect on the Laplace refining process, which means that the simulation results are not affected. If your CAD program cannot export STL, there is still a good possibility that some utility or plug-in exists that can convert your CAD format into STL. We are open to the possibility of natively adding support for other formats.

On the next page is some fun we had in using a shopping cart CAD model to simulate a non-ideal grid for ion optics studies. Notice that the potential energy surface inside the cage is roughly constant except for the field propagation effects through the cage holes and top.



**Figure #4 - (1) - Original CAD model, (2) - Model imported into SIMION with ion optics studies - 3D View, (3) - Model imported into SIMION with ion optics studies - X-Z View, (4) - potential energy map inside the cage.**  
 (STL source: <http://www.3dcadbrowser.com>)

## SL Compiler

The second major feature of SIMION SL is a high-level language to replace the SIMION PRG language. SIMION provides the PRG user programming language so that you can really customize the behavior and logic of your simulation: oscillate electrode voltages, perturb or randomize ion trajectories, perform calculations, collect data, and respond to events. However, the PRG language is somewhat archaic, as many users would likely prefer to program in a language resembling C or Pascal rather than assembly or Forth. The main features of the SL language are given below and are largely what is expected from a procedural language:

- Write SIMION custom programs in a high-level language.
- Infix expressions:  $x + \cos(2 + x * y) / \log(n + 1)$
- Array syntax:  $x[y + 2] = y[3 * n / 2]$
- Custom subroutines, recursion, multiple return values
- Loops: for, while
- Conditionals and Boolean logic: if, functional-if,  $(x > 2 * y)$  or not  $(x = 0)$  and  $y > 2 + \cos(x)$

- List assignment:  $(x, y, z) = \text{rect3d\_to\_polar3d}(a, b, c)$
- Utility functions: min, max, ceil, floor
- Import/include mechanism
- Compiles to PRG code formatted for human-readability.
- SL Remote: Call subroutines in a remotely running C++ program from SL. (support for other languages can be added upon request) \*\*

An example of SIMION SL code is provided on the next page. This program is functionally equivalent to SIMION's RANDOM.PRG example, where the initial kinetic energy of a series of ions is randomized uniformly, and the initial velocity direction is randomized by a given angle within the vertex of a cone. In fact, the SIMION SL compiler translates SL code directly into PRG code for use by SIMION and can be executed in conjunction with existing PRG programs.

```

=====
# random.sl - randomize ions
#
# The program demonstrates how to apply randomization to the
# kinetic energies and velocity directions of ions originating in
# the potential array associated with this program.
#
# The NEW KE of each ion is randomized by a factor of
# +- (percent_energy_variation %) with respect to the defined value.
#
# The NEW DIRECTION of each ion is randomized within a cone of revolution
# around the defined velocity direction. The angle of this cone
# is taken to be +- cone_angle_off_vel_axis degrees.
#
# Upon compilation, this SL program can be used as an exact replacement
# for the RANDOM.PRG program in the _Random example of SIMION 7.0.
=====

===== variables

# energy variation (in percent), must be in the interval [0, 100]
adjustable percent_energy_variation = 50

# cone angle (in degrees), must be in the interval [0, 180]
adjustable cone_angle_off_vel_axis = 90

===== subroutines

# Initialize ion's velocity and direction at the start of simulation.
sub initialize

# First, let's check user input...
# Ensure 0 <= percent_energy_variation <= 100.
percent_energy_variation = min(abs(percent_energy_variation),100)
# Ensure 0 <= cone_angle_off_vel_axis <= 180.
cone_angle_off_vel_axis = min(abs(cone_angle_off_vel_axis),180)

# Now, let's do the actual randomization...

# Convert original ion velocity to 3-D polar coordinates.
(speed, az_angle, el_angle)
= rect3d_to_polar3d(ion_vx_mm, ion_vy_mm, ion_vz_mm)

# Randomize ion's KE.
new_ke = speed_to_ke(speed, ion_mass)
* (1 + (percent_energy_variation / 100) * (2 * rand() - 1))
# Convert new KE back to ion speed, and set it.
speed = ke_to_speed(new_ke, ion_mass)

# Now, to randomize the ion velocity direction, we first do the below
# to make the ion's possible random velocity directions fill a solid cone
# with vertex at the origin and axis oriented along the positive y-axis.
# The angle that the cone side makes with the cone axis will be
# the cone_angle_off_vel_axis value.

# randomize elevation angle: (90 +- cone_angle_off_vel_axis)
new_el = 90 + cone_angle_off_vel_axis * (2*rand()-1)
# randomize azimuth angle: (0 +-90)
new_az = 90 * (2*rand()-1)

# Now that we generated this randomized cone, we will rotate it
# so that the expected ion velocity direction matches the ion's
# original velocity direction.

# Convert to rectangular velocity components.
(x, y, z) = polar3d_to_rect3d(speed, new_az, new_el)
# Rotate back to defined elevation.
(x, y, z) = elevation_rotate(-90 + el_angle, x, y, z)
# Rotate back to defined azimuth.
(ion_vx_mm, ion_vy_mm, ion_vz_mm) = azimuth_rotate(az_angle, x, y, z)
endsub

```

## Miscellaneous

So what else can the SIMION SL Toolkit do? Some are hinted in the list of components given in the introduction. SIMION SL also includes various GUI functions and programming libraries for manipulating and extracting field data from SIMION potential arrays. For full details, check out our web site, [www.simion.com](http://www.simion.com). We have recently published a number of articles in the "Documentation" section describing how to get more out of SIMION with and without SIMION SL.

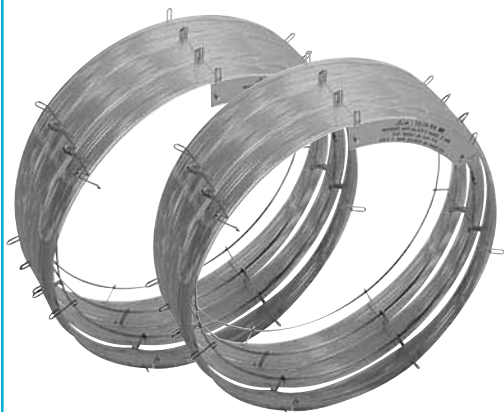
In fact, the [www.simion.com](http://www.simion.com) web site has been resurrected just this past year, and much of the content is less than a year old. In part with the online discussion group and the more extensive online resources, we're working to establish a community around SIMION so that you too can get the most out of SIMION.



# Agilent/J&W Columns

*Exclusive Offer From S.I.S.*

**Purchase Two or More  
Agilent/J&W Columns**



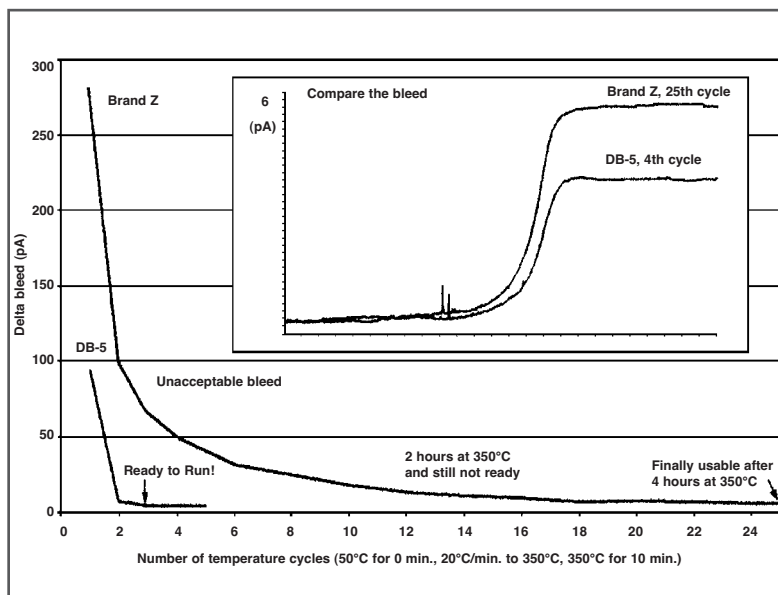
**... and Receive A  
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Column Cutter**



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## Lowest Bleed

Agilent's MS-grade columns are specifically engineered for low bleed, high thermal stability and excellent inertness. With the lowest bleed level, the best inertness for acids/bases/mixed functional compounds, and tightest column-to-column reproducibility, Agilent GC columns are of higher quality and perform better than any other columns on the market.



\*One per Customer. Limited time offer. Not For Use With Other Promotional or Discount Offers.

Offer Expires August 1, 2004 or while supplies of Shortix Plus™ Inventory last.

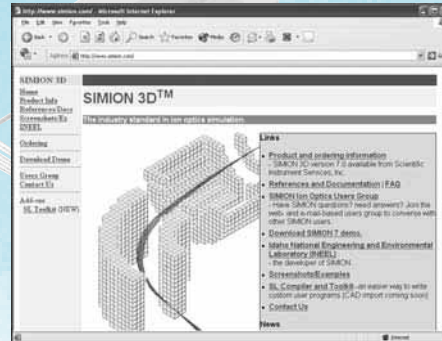
# SIMION.COM

A **NEW** Web Site Dedicated to Serving the SIMION Community.  
It hosts our new SIMION Users Discussion Group

<http://www.simion.com>

## Features:

- Discussions among SIMION users via the web and e-mail
- Product Information
- Downloads
- Articles

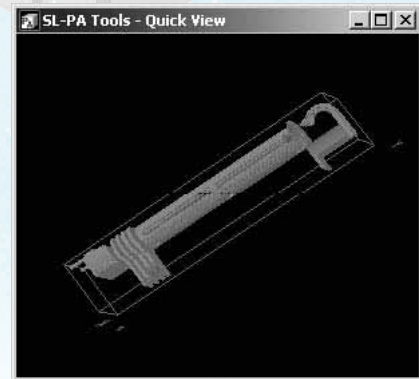


**NEW**

## SIMION SL Toolkit

“SL” Expands the Capabilities of SIMION 3D Ion Optics Modeling Software with

- **The SL Compiler** - write your user programs in the high-level SL language or call remote C++ code.
- **Potential Array Tools**
  - transfer CAD models to/from SIMION.
  - extract data from refined potential arrays
  - manipulate potential array files in C++/Perl/Python.
- **Additional utilities.**



Part No.	Description
SIMIONSL2	SIMION SL Toolki

Scientific Instrument Services  
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Ringoes,NJ 08551

Bulk Rate  
US Postage  
**PAID**  
Permit No.388  
Somerville, NJ

