Method for Improved Accuracy with Simion for Models having Curved Electrode Surfaces

David G. Welkie, Analytica of Branford, Inc., Branford, CT 06405

OVERVIEW

- The Simion potentials 'refinement' process [1] employs finite differences methods to numerically solve the Laplace equation for potentials at discrete points of an orthogonal grid, using electrode surface geometry and potentials as boundary conditions.
- However, curved or slanted electrode surface contours can only be represented approximately by an orthogonal grid, which limits the accuracy of the calculated potentials [1,2].
- We introduce a modified approach to defining boundary conditions that provides improved accuracy, particularly when an electode surface is an equipotential contour of an analytical potential function, as in many energy and mass analyzers.
- Results are presented here for models of 3D ion traps and quadrupole mass filters that demonstrate substantial improvements with the new method.

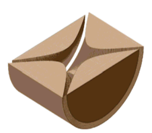
METHODS

- Simion potential array ('pa') files are defined for a geometry in a conventional manner.
- Potentials at grid points representing a curved electrode surface are each 'corrected' individually according to the known analytical potential distribution function, thereby compensating for the surface grid points' spatial offsets from the real electrode surface.
- The resulting modified 'pa' files are 'refined' with Simion as usual to determine non-electrode potentials.
- The modified potentials of the individual curved surface grid points are returned to the potential of the electrode, enabling Simion to subsequently scale the calculated non-electrode potentials.
- This technique is referred to here as the 'Corrected Individual Surface Points' method, or, the 'CrISP' method.

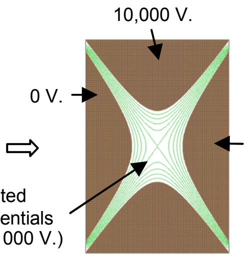
'IDEAL' 3D ION TRAP

2D cylindrical symmetry

R_0 = 10.0 mm

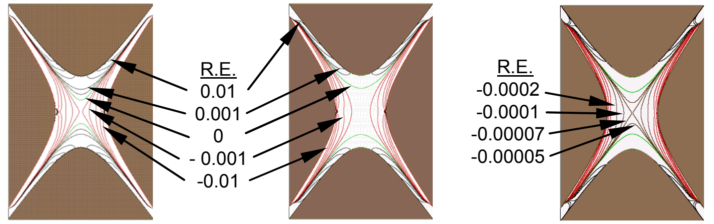


Conventional Simion refinement of potentials using a 'Converence Objective' ('CO') = 1×10^{-7} ⇨



$$\text{Relative Error ('R.E.')} = \frac{\text{calculated potential – theoretical potential}}{\text{theoretical potential}}$$

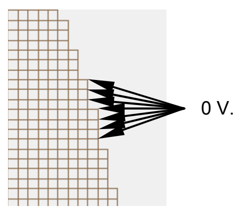
Relative Error vs. Grid Spacing (Conventional Methods):



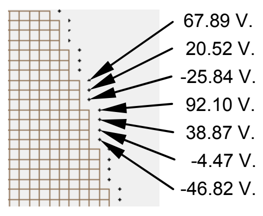
gu = 0.100 mm | gu = 0.020 mm | gu = 0.005 mm

➡ ~10X improved accuracy from 20X smaller grid spacing suggests that computational errors result from imperfect electrode surface discretization.

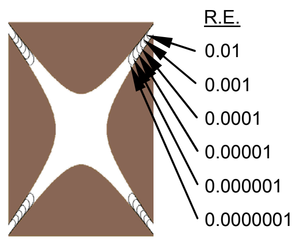
Application of the 'CrISP' Method:



Conventional Model: Portion of left end cap electrode model with gu = 0.10 mm



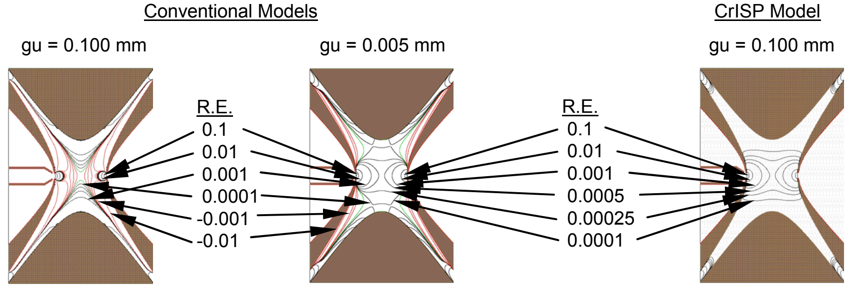
CrISP Model: Correction of potentials at individual surface points, based on the surface points' locations and the theoretical potential distribution function



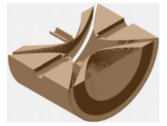
Relative errors after Simion refinement of the CrISP model, **demonstrating orders-of-magnitude improvement**, compared to conventional models even with 20X finer grid spacing

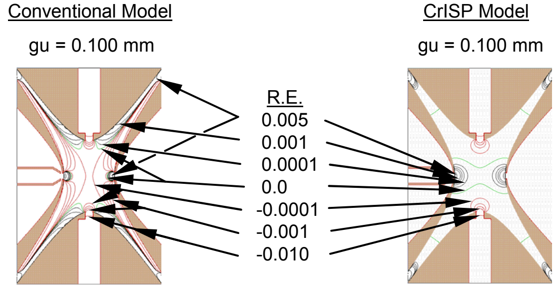
'PRACTICAL' 3D ION TRAPS with ACCESS HOLES

End cap holes - cylindrical symmetry allows conventional 2D modeling with a gu of 0.005 mm or less. Again, however, better accuracy is provided by a CrISP model with a 20X larger gu of 0.100 mm.



Ring electrode holes - cylindrical symmetry is destroyed, so a full 3D planar array model is necessary. Simion (7.0) maximum of 50 million grid points limits gu to >~0.10 mm, even with Simion planar 'mirroring'.

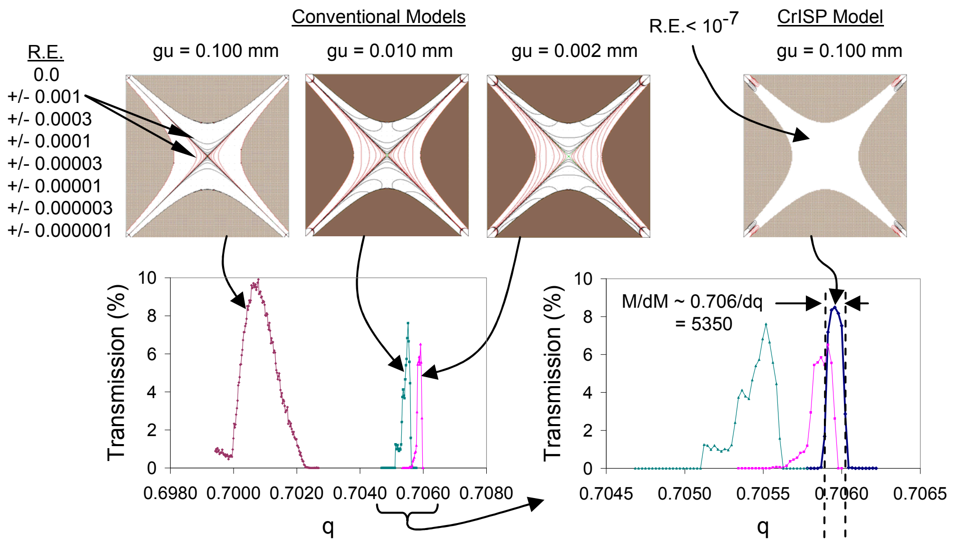




➡ Conventional approach generally provides good accuracy. However, the CrISP approach uniquely allows high accuracy to be maintained even when finer grid spacings are not possible due to array size constraints, as with full 3D planar models.

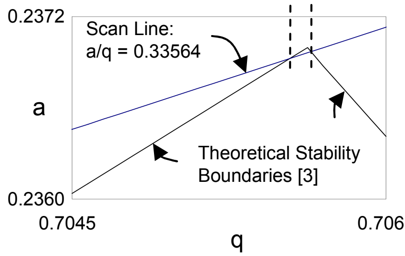
'IDEAL' QUADRUPOLE MASS FILTER

2D planar symmetry; R_0 = 4.10 mm

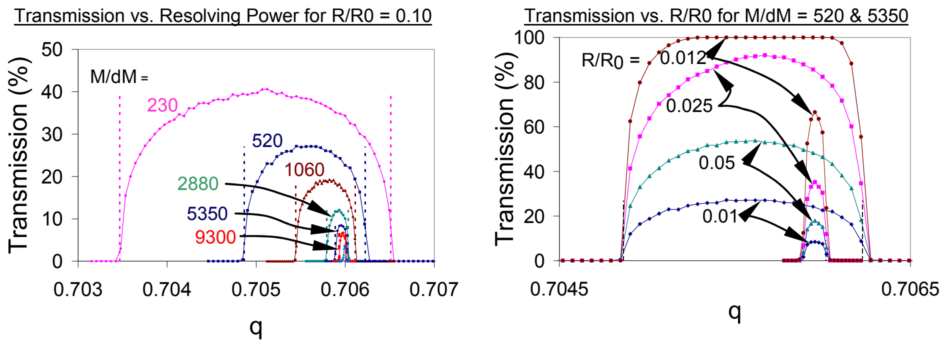


Mass Peak Profiles:

- M/z = 322
- Initial K.E.= 0.1 eV; No angular spread
- 100 ions randomly distributed within R = 0.1 R_0
- @ 90 Initial RF phases from 0 to π (9000 ions/point)
- Quadrupole 'length' = 200 mm (816 cycles @ 1 MHz)



CrISP 2D Quadrupole Model with gu = 0.10 mm


Transmission vs. Resolving Power for R/R0 = 0.10

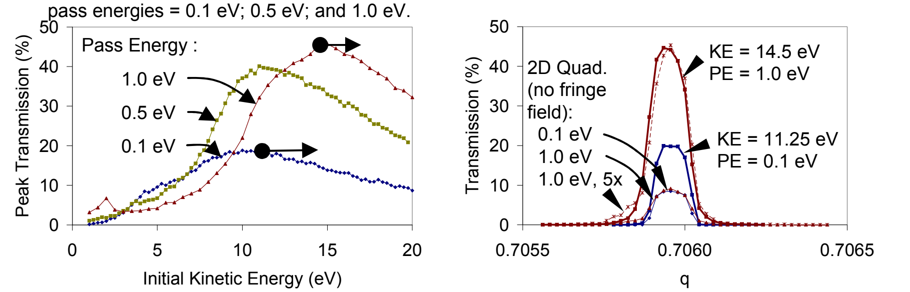
Transmission vs. R/R0 for M/dM = 520 & 5350

➡ Computational accuracy of ideal 2D quadrupole potentials is much better for CrISP model using 0.1 mm gu, compared to conventional models using 0.002 mm gu.

➡ Trajectory calculations with CrISP models with gu = 0.100 mm exhibit trajectory stability characteristics consistent with analytical theory [3], in contrast to conventional Simion models.

HYPERBOLIC QUADRUPOLE MASS FILTER WITH ENTRANCE APERTURE

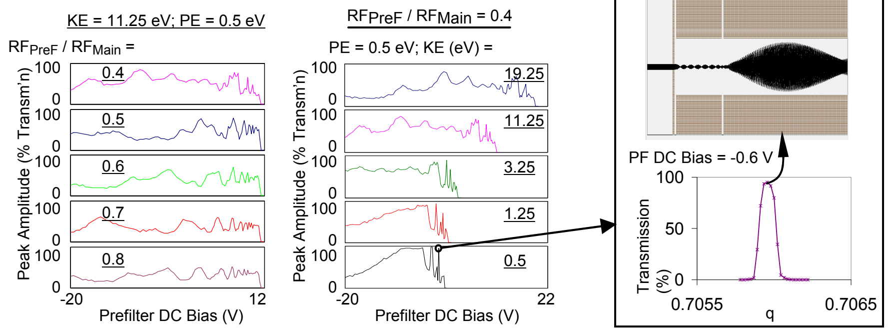
3D Potential Array = 2 mm entrance aperture & 43 mm long quadrupole entrance portion, followed by
2D Potential Array = 157 mm long 2D quadrupole (Total quadrupole length = 200 mm).
CrISP applied to all hyperbolic surfaces. Trajectory Calculations: Same initial trajectory parameters as previous. (R/R0 = 0.10 only). Recorded peak amplitude vs. initial ion energy (& quad. offset) for pass energies = 0.1 eV; 0.5 eV; and 1.0 eV.



➡ Entrance aperture fringe field improves transmission efficiency relative to ideal 2D quadrupole, provided the initial ion energy is optimized. Leading edge peak tail is also improved.

HYPERBOLIC QUADRUPOLE MASS FILTER WITH ENTRANCE APERTURE AND PREFILTER

3D Potential Array: Added 25 mm long prefilter between grounded entrance aperture and quadrupole. CrISP applied to all hyperbolic surfaces. Trajectory Calculations: Same initial parameters as previous. Recorded peak amplitude vs. prefilter DC offset.



➡ Transmission efficiency oscillates with both prefilter DC bias and applied RF amplitude, due to changes in each causing beam noding & anti-noding at the prefilter/quadrupole interface region.

➡ Multiple conditions of prefilter DC bias and RF amplitude provide significant transmission improvements over quadrupoles without a prefilter, but at the cost of increased complexity.

CONCLUSIONS

❖ A modified approach to electrode modeling ('CrISP') has enabled more accurate calculation of potentials with Simion when curved electrode contours are equipotential surfaces of a known potential distribution.

❖ The improved accuracy results in close agreement between numerical calculations and analytical theory, and has allowed elucidation of fringe field effects using otherwise standard Simion functionality (although ion energy & angular dispersions have not yet been included).

REFERENCES

1. Dahl, D.A., Int. J. Mass Spectrom. 200, 3-25 (2000).
2. Zouros, T.J.M., et. al., Int. J. Mass Spectrom. 261, 115-133 (2007).
3. Dawson, P.H., "Quadrupole Mass Spectrometry and Its Applications", Elsevier, Amsterdam (1976).