

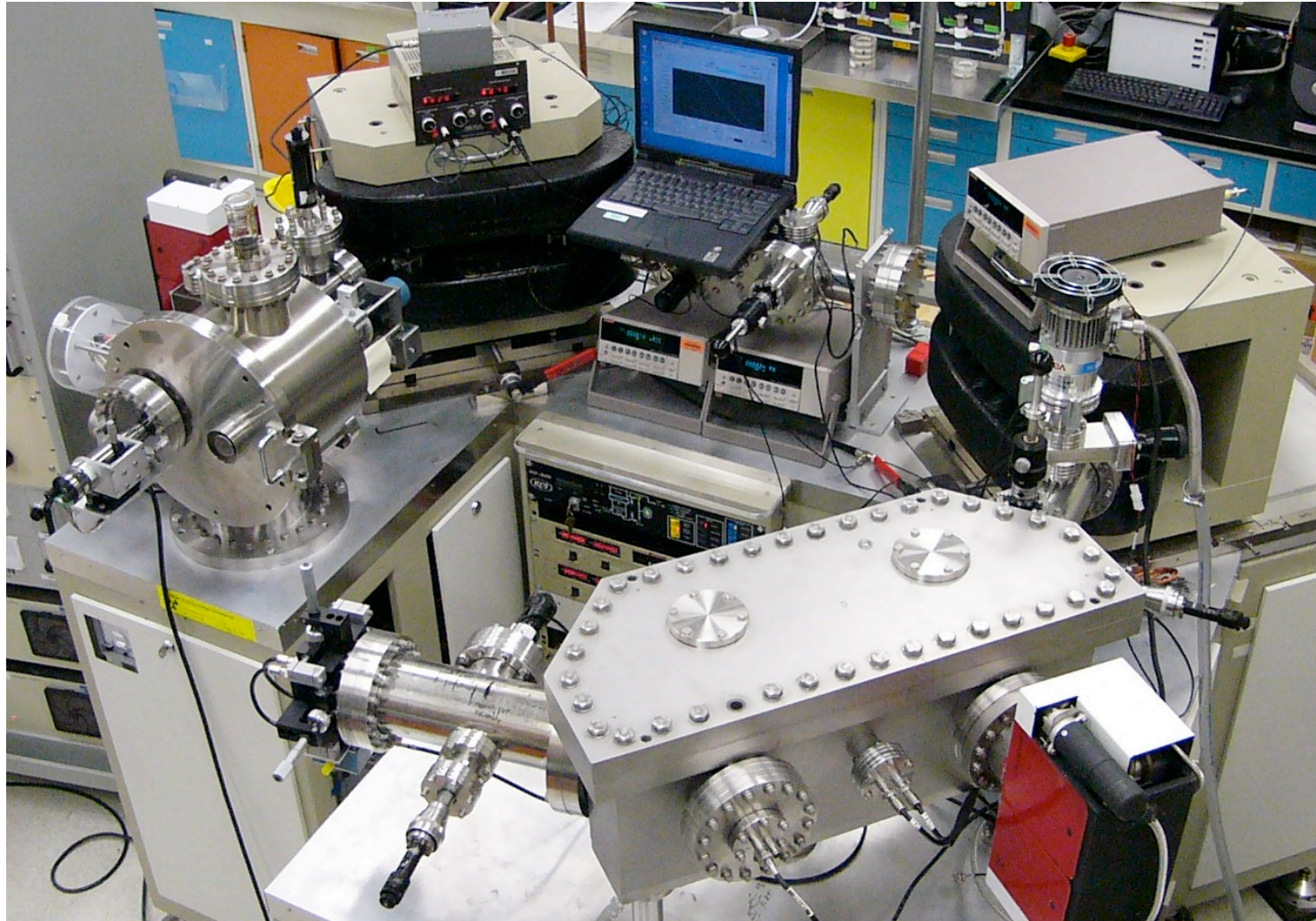
Ion Optics Simulations

- What it is.
- How it's useful.
- The SIMION ion optics software.
 - How it works.
 - Limitations and cautions
 - Demonstrations and examples
 - A little hands on exploring

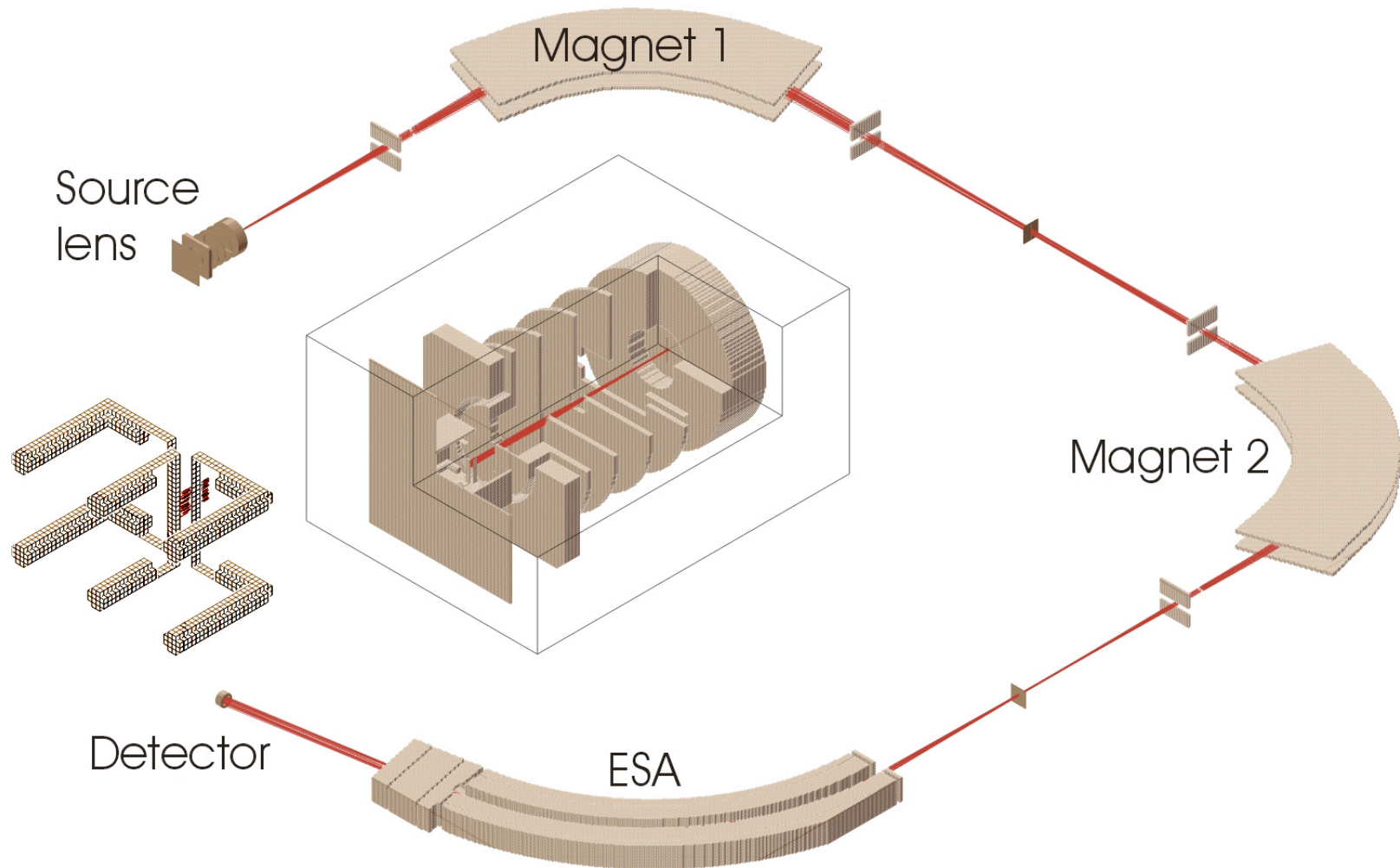
Ion Optics Simulations

Mathematical and numerical models of electric and magnetic fields and the effect of these fields on charged particles within them.

Triple Sector TIMS



Triple Sector TIMS Model

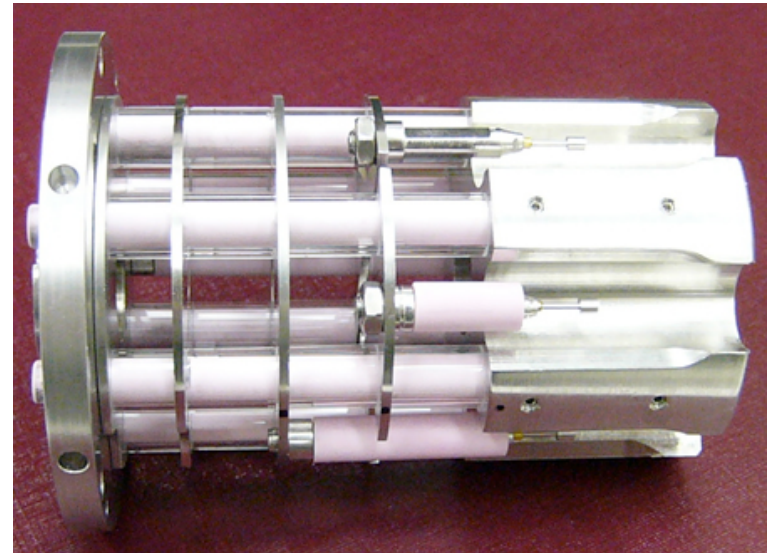
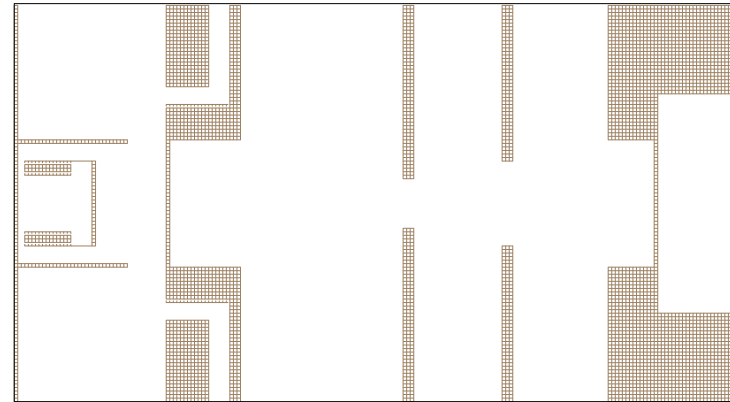
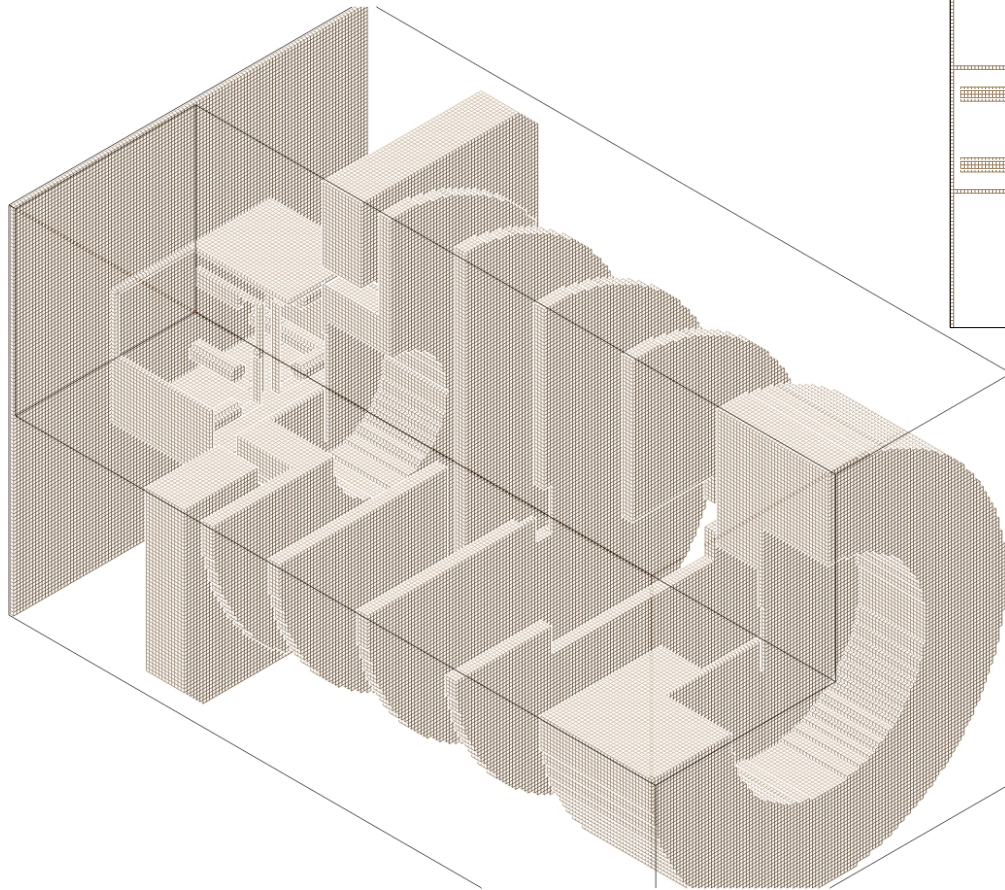


Simulations

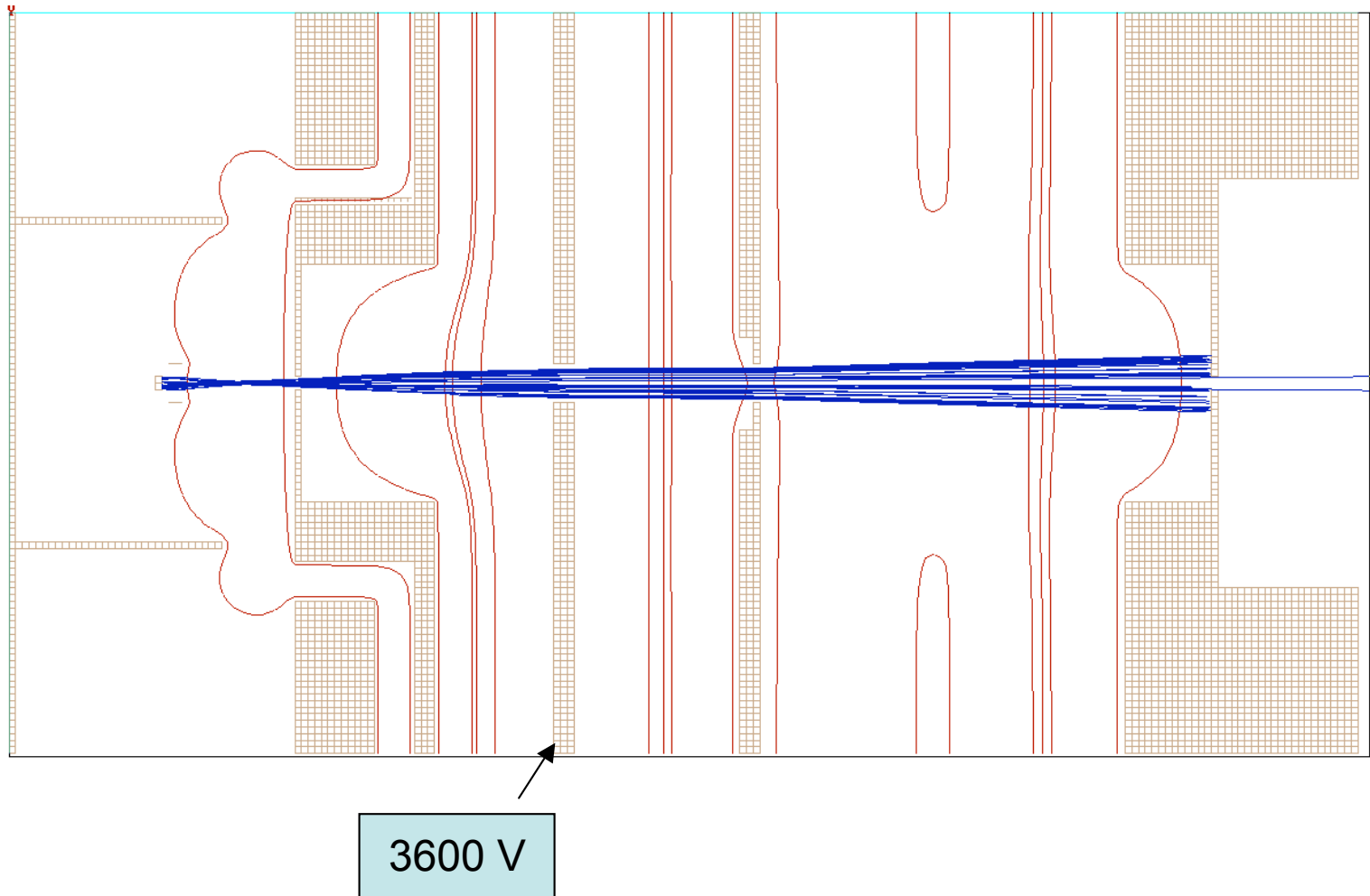
Help us:

- Develop an understanding of how our instruments work
 - optimize their performance and
 - understand the data they generate.
- Develop some intuition useful for
 - guiding new developments and
 - trouble shooting.
- Explore new ideas easily with little cost.

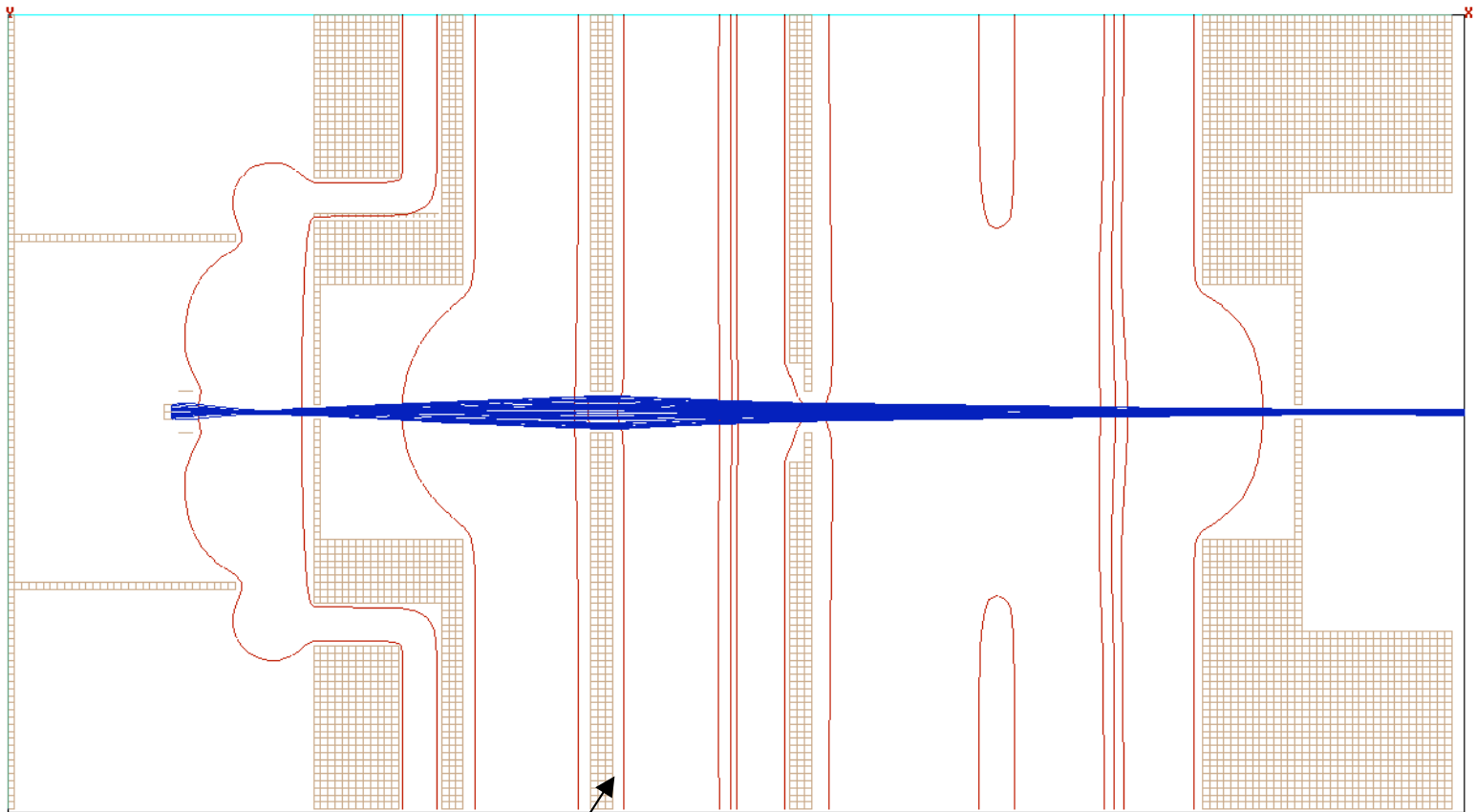
Ion Lens Tuning



Lens Tuning – Poor Signal

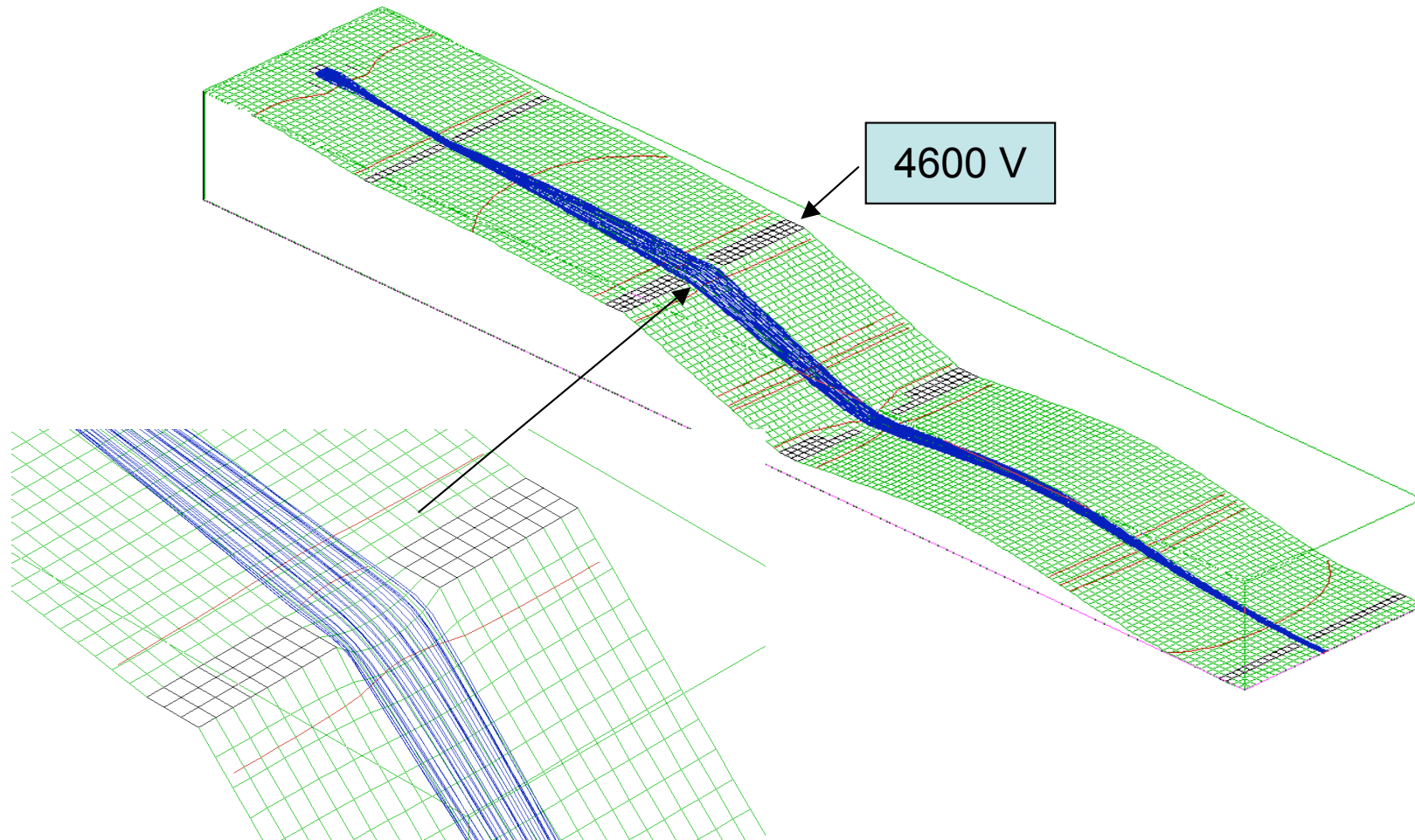


Lens Tuning - Better Signal

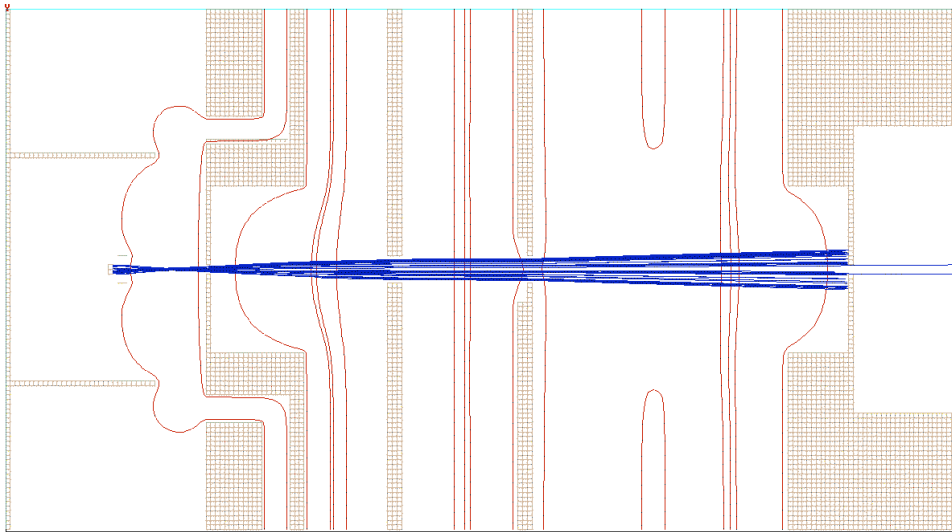


4600 V

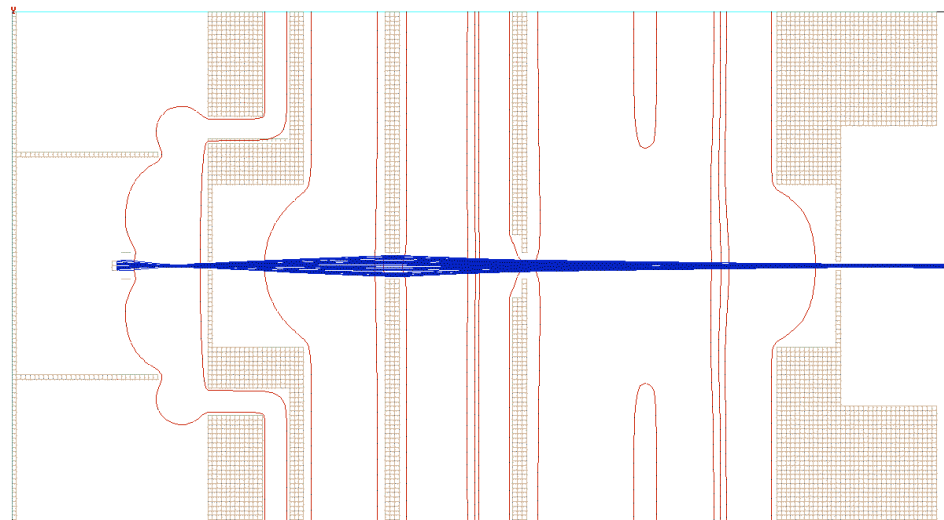
What's Happening?



Model –Builds Intuition



Gaining an understanding of what we are doing to the ions when we fiddle with the knobs.



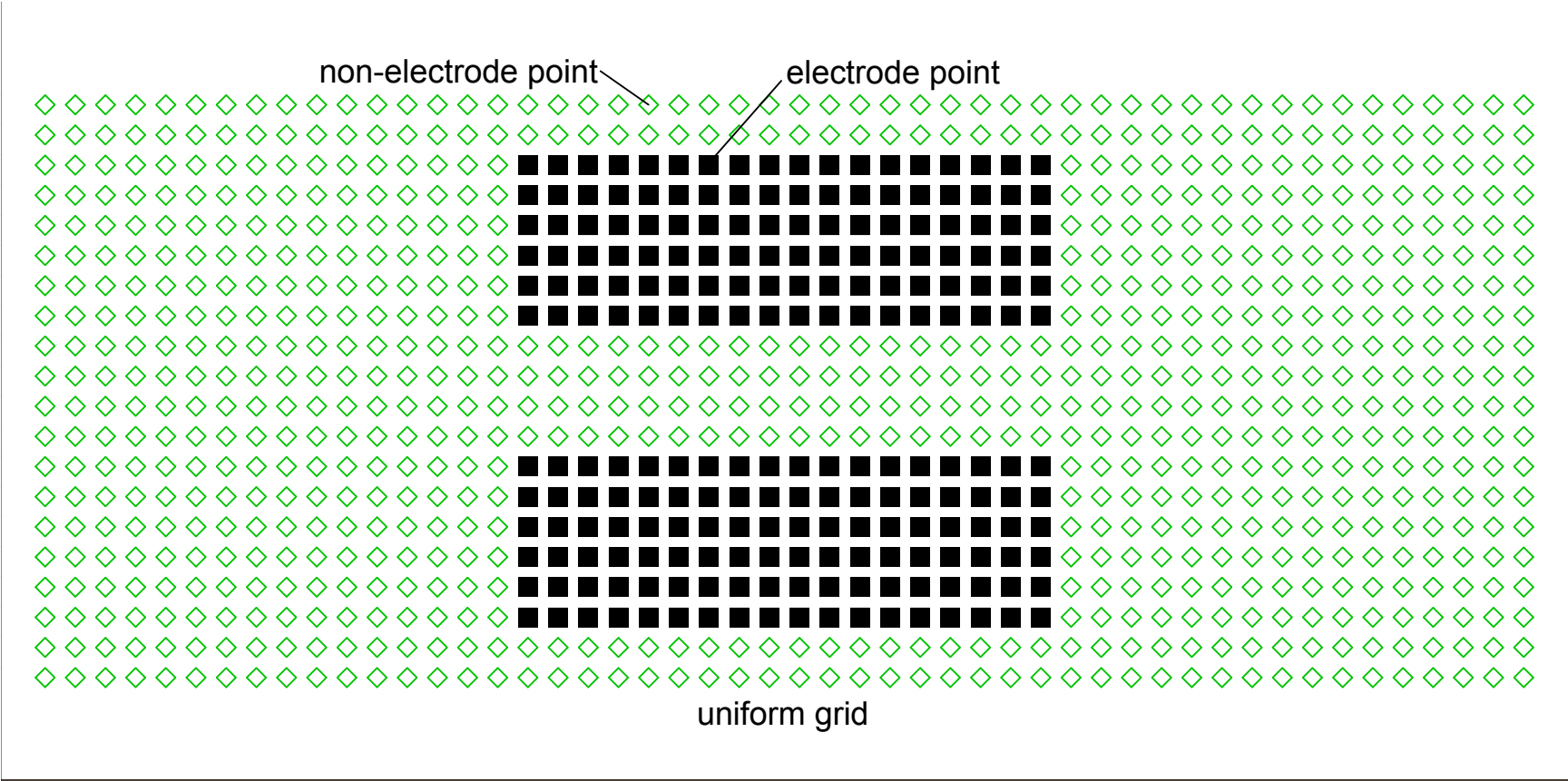
SIMION 3-D

- One of several computer programs for ion optics modeling.
 - Developed by David Dahl at the Idaho National Laboratory.
 - Currently available from Scientific Instrument Services – allowing us free use of the program for this course.

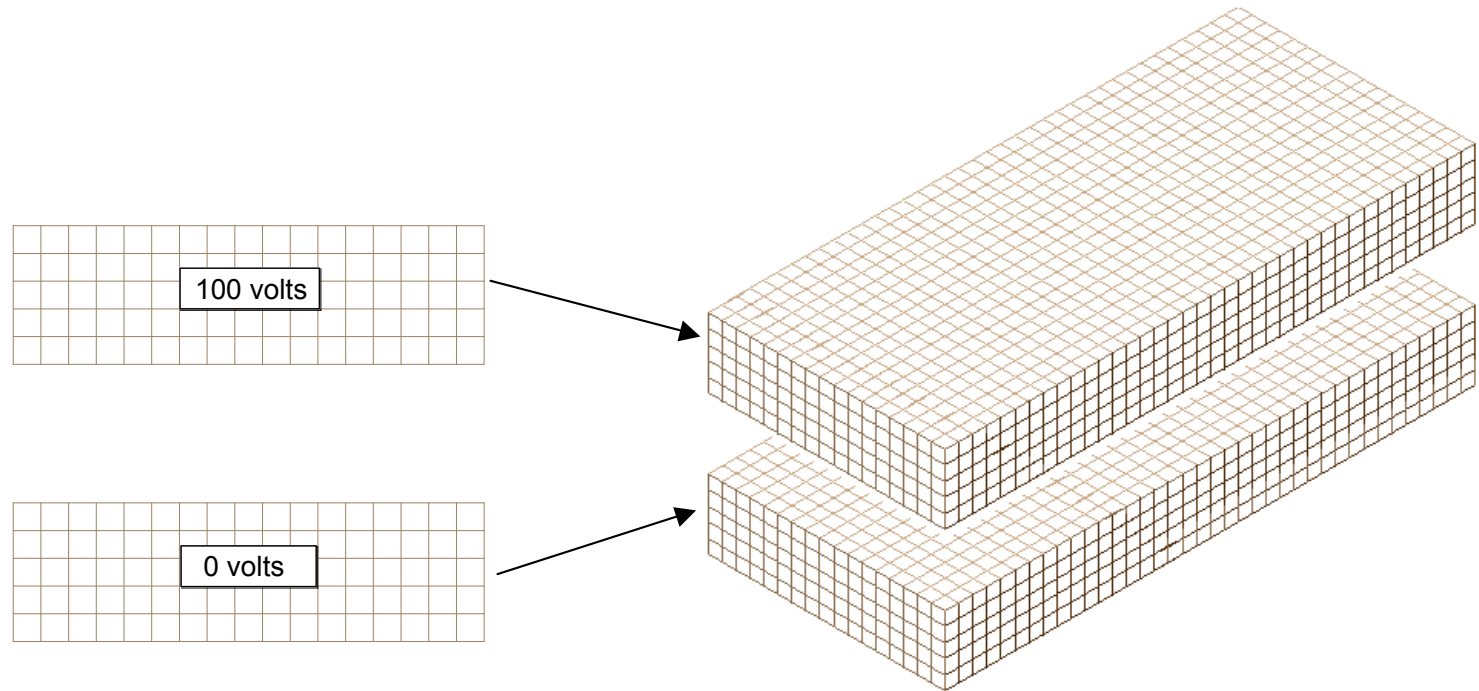
How does it work?

- The user defines the physical geometry of the components in the system based on a uniform grid and sets the potentials (electric and magnetic) on the electrodes.
- The program numerically calculates the electric and magnetic fields in the spaces between the electrodes, determining the potential at each grid point.

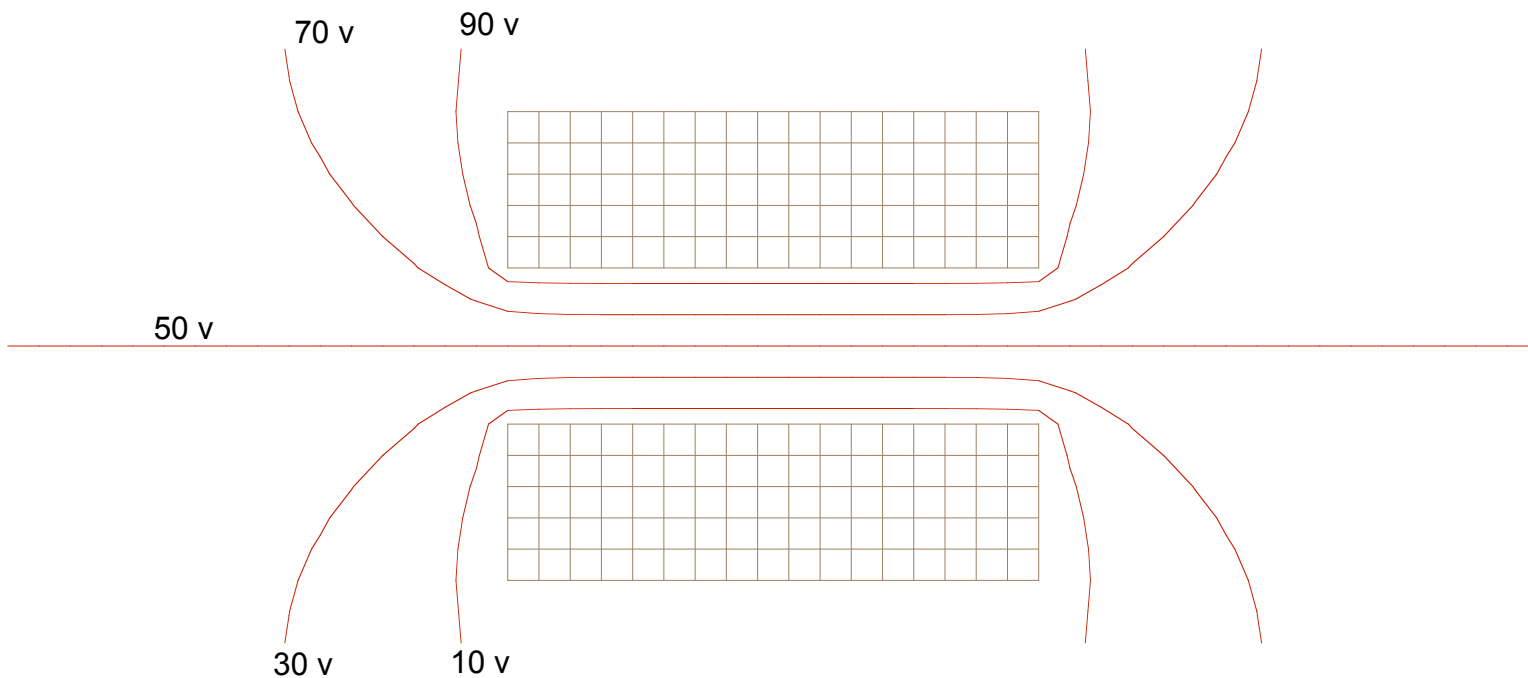
Grid Geometry



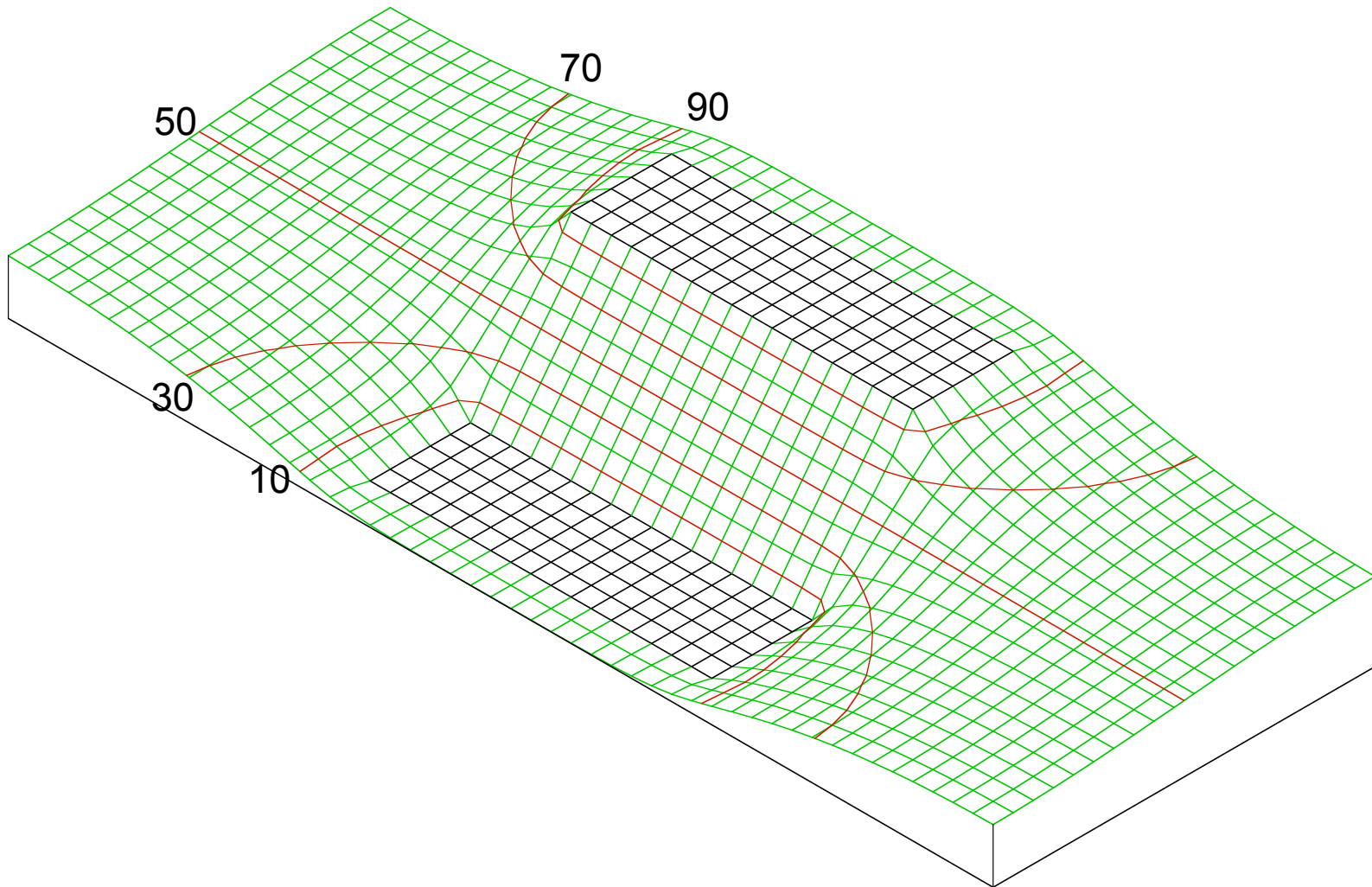
Grid Geometry



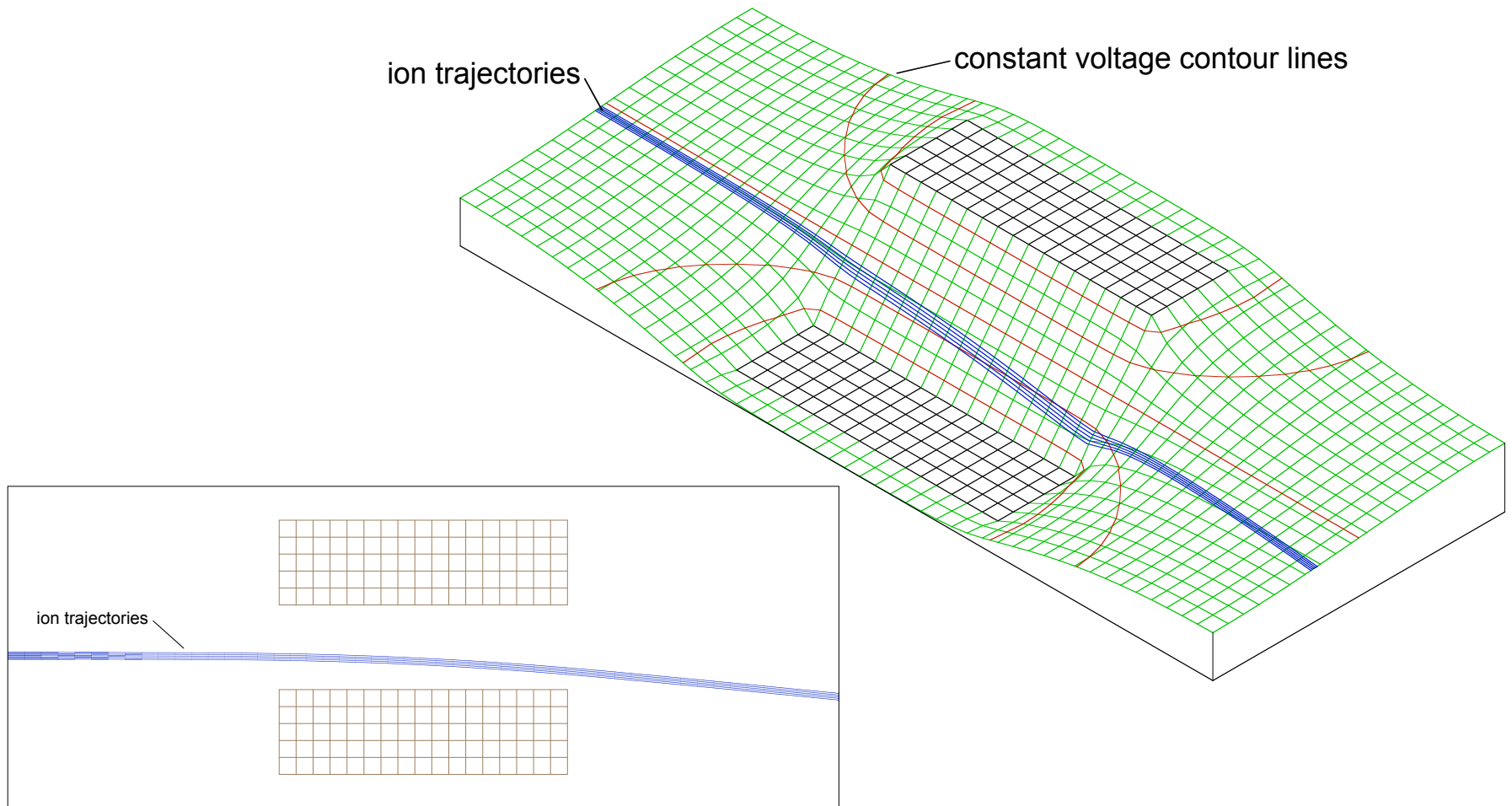
Voltage Map Created By “Refining” the Array



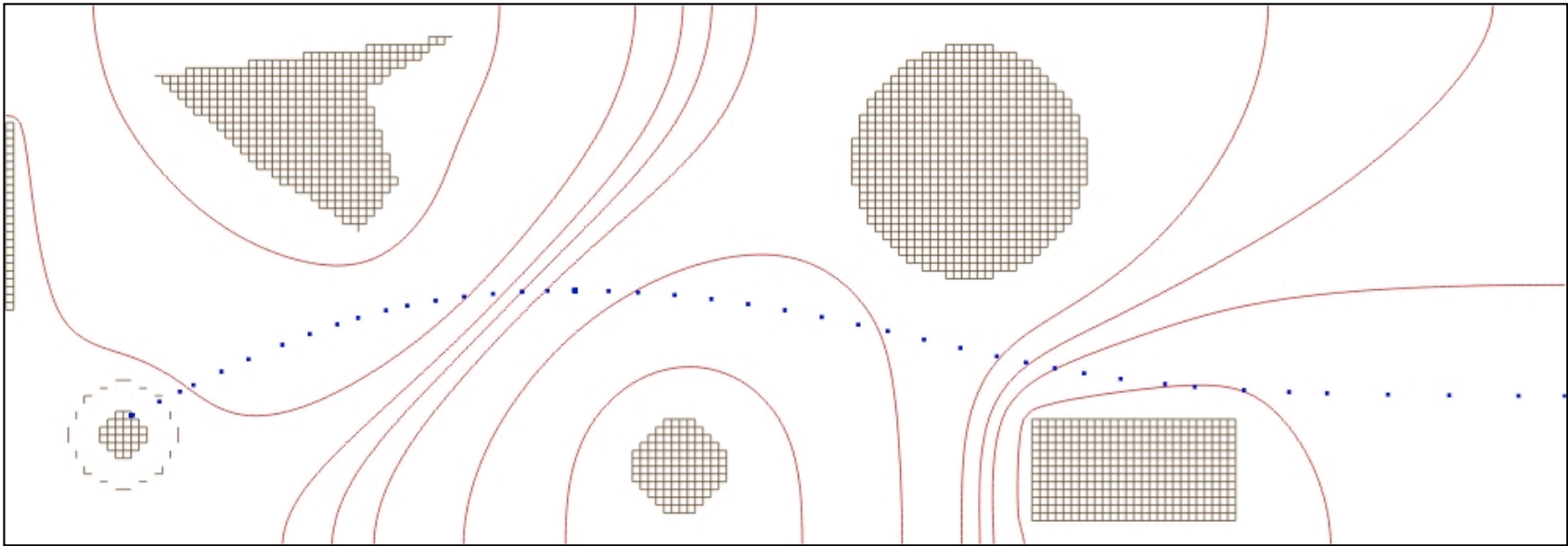
Potential Energy Surface



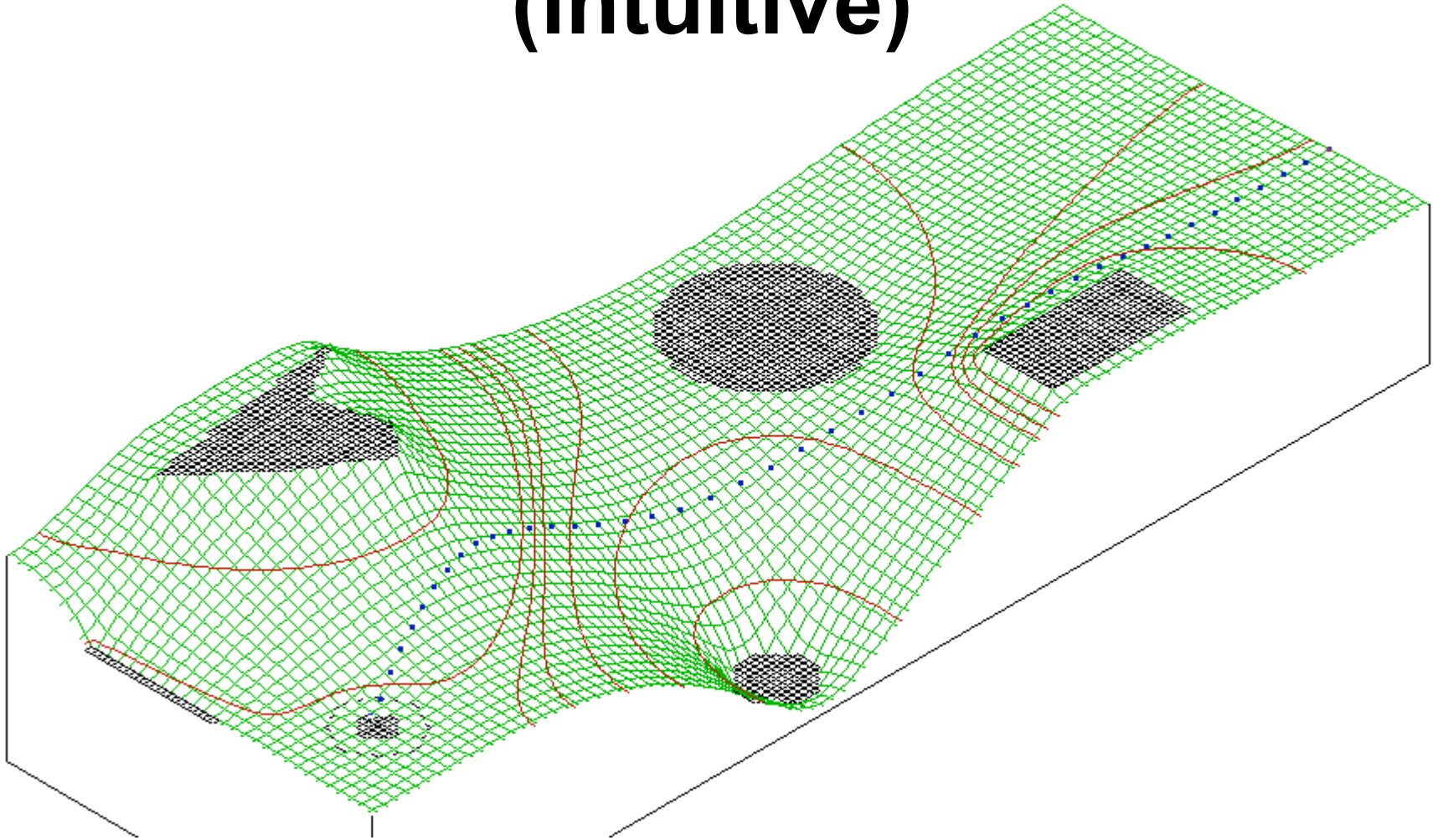
Ion Trajectories



Contour Map (non-intuitive)



Relief Map (intuitive)



Analytical Field Definition

If we know an analytical function that describes the field, we can apply that to the array area in place of the refined grid array when calculating ion trajectories.

- Ignores any perturbations that may be present
 - Asymmetries
 - Off-axis components
- Useful for checking fidelity of the refined grid.

Refining the Grid

- The electrostatic or magnetic field potential at any point within an electrostatic or static magnetic lens can be found solving the Laplace equation with the electrodes (*or poles*) acting as boundary conditions.
- The Laplace Equation

$$\nabla^2 V = 0$$

- The Laplace equation constrains all electrostatic and static magnetic potential fields to conform to a zero charge volume density assumption (*no space charge*).

Refining the Grid

- Poisson's Equation Allows Space Charge

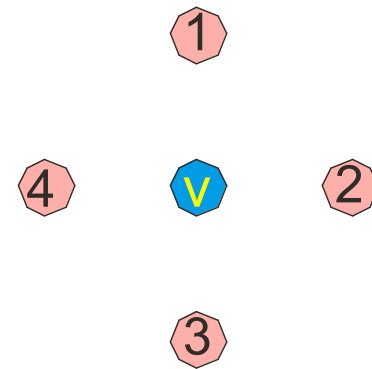
$$\text{DEL}^2 V = - \rho / \epsilon$$

- Poisson's equation allows a non-zero charge volume density (*space charge*).
- ***SIMION does not support Poisson solutions to field equations. It does however employ charge repulsion methods that can estimate certain types of space charge and particle repulsion effects.***

The Nature of Solutions to the Laplace Equation

- The Laplace equation defines the potential of any point in space in terms of the potentials of surrounding points.
- For example, Laplace equation is satisfied (*to a good approximation in 2D*) when the potential of any point is **estimated** as the average of its four nearest neighbor points:

- $V = (V_1 + V_2 + V_3 + V_4) / 4$



Refining the Array

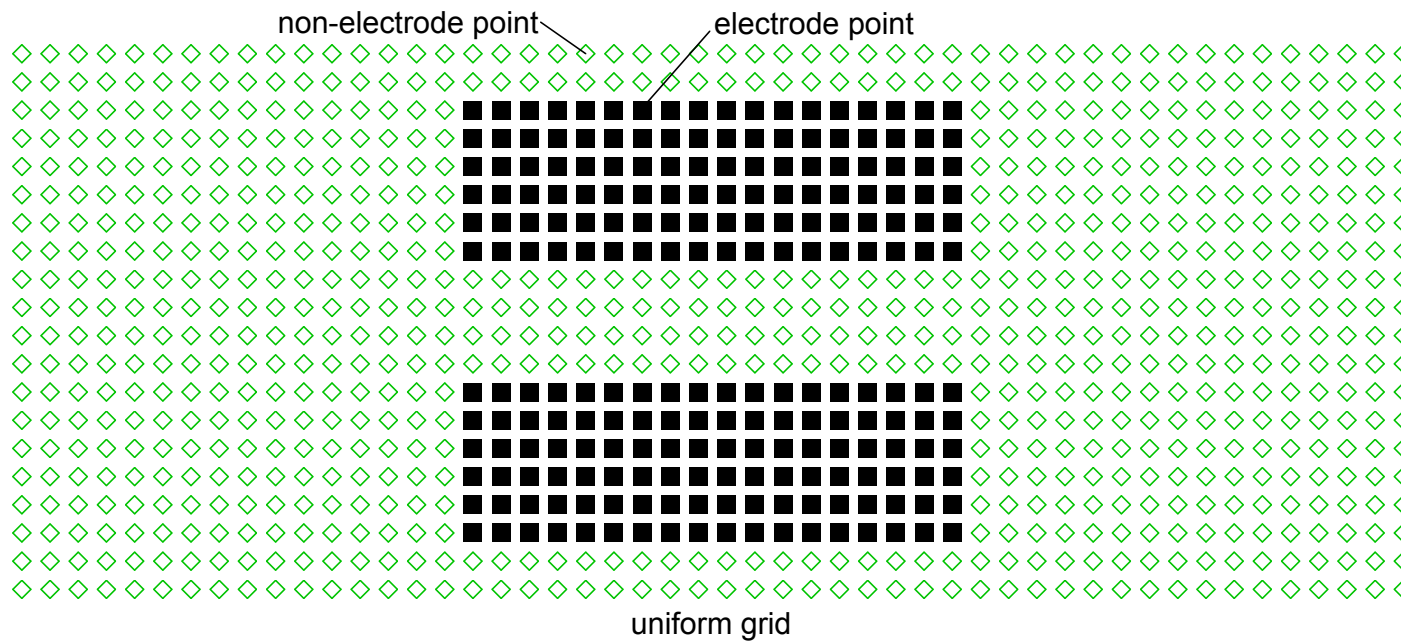
1

2

3

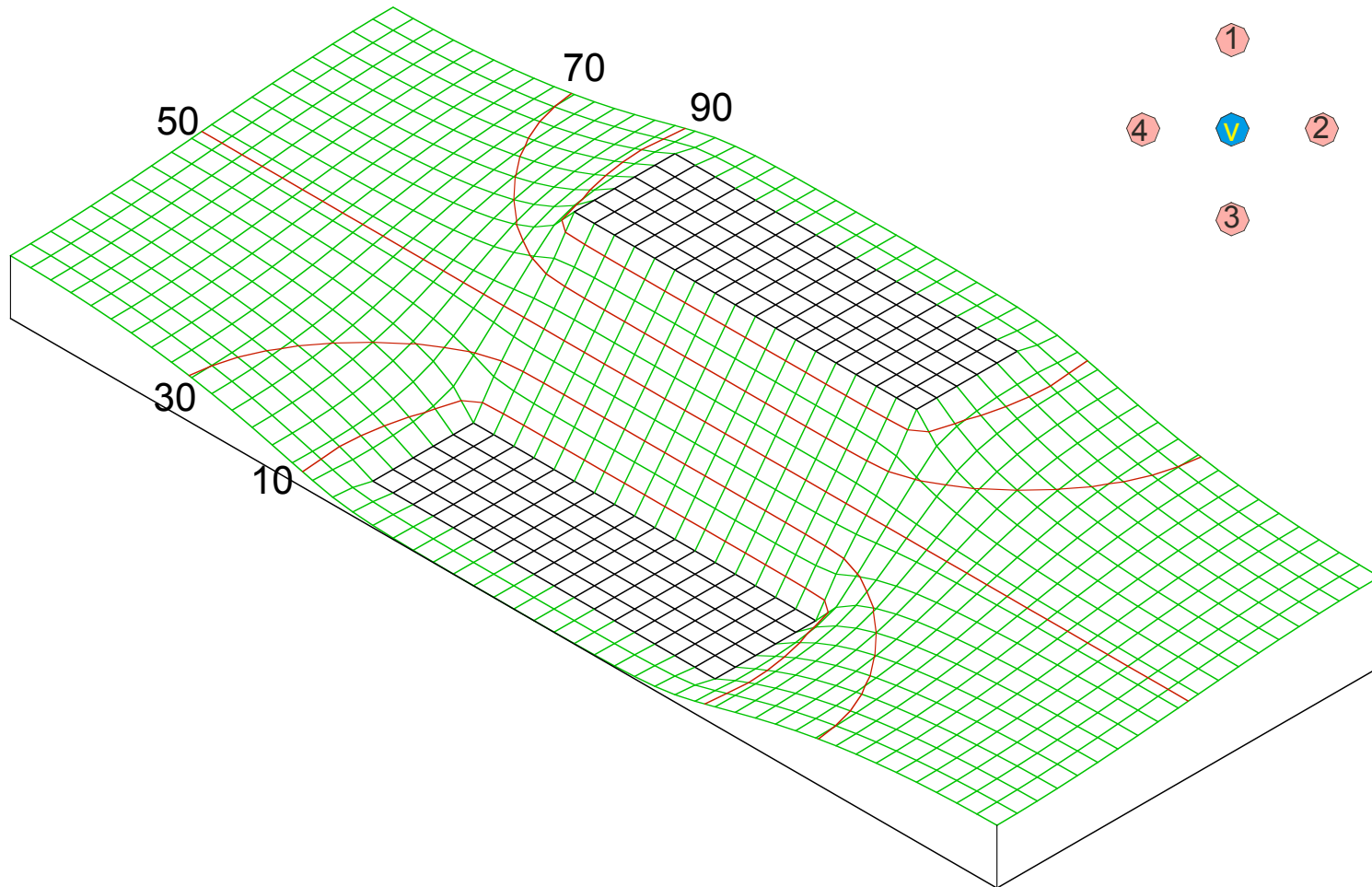
4

V



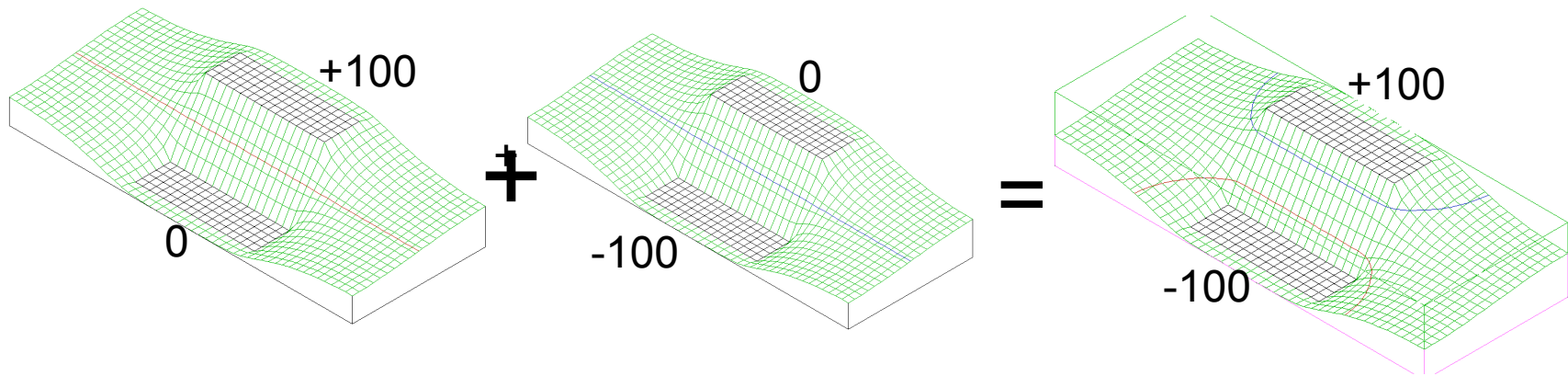
Refining involves starting at the left side, and computing the average for each point using its four neighbors; repeating this process until the difference between the current and the previous value is less than some set limit (for example, $1 \text{ e-}7$). SIMION employs a host of tricks to speed up this process, not discussed in this lecture.

The Refined Array



The Nature of the Laplace Equation

- Solutions for overlapping arrays are additive.

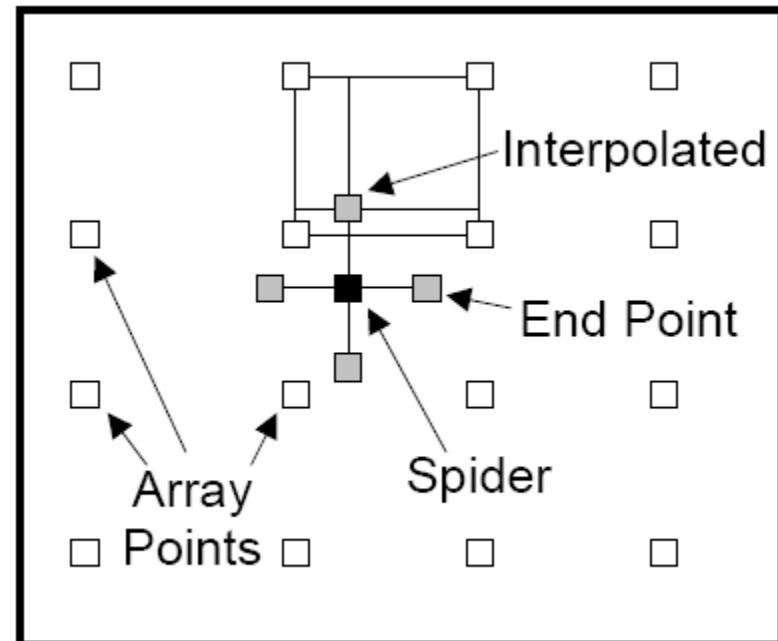


Enables a method for quickly changing the potential on individual electrodes without having to re-refine the entire array – this is called Fast Adjust in SIMION.

Calculating Ion Trajectories

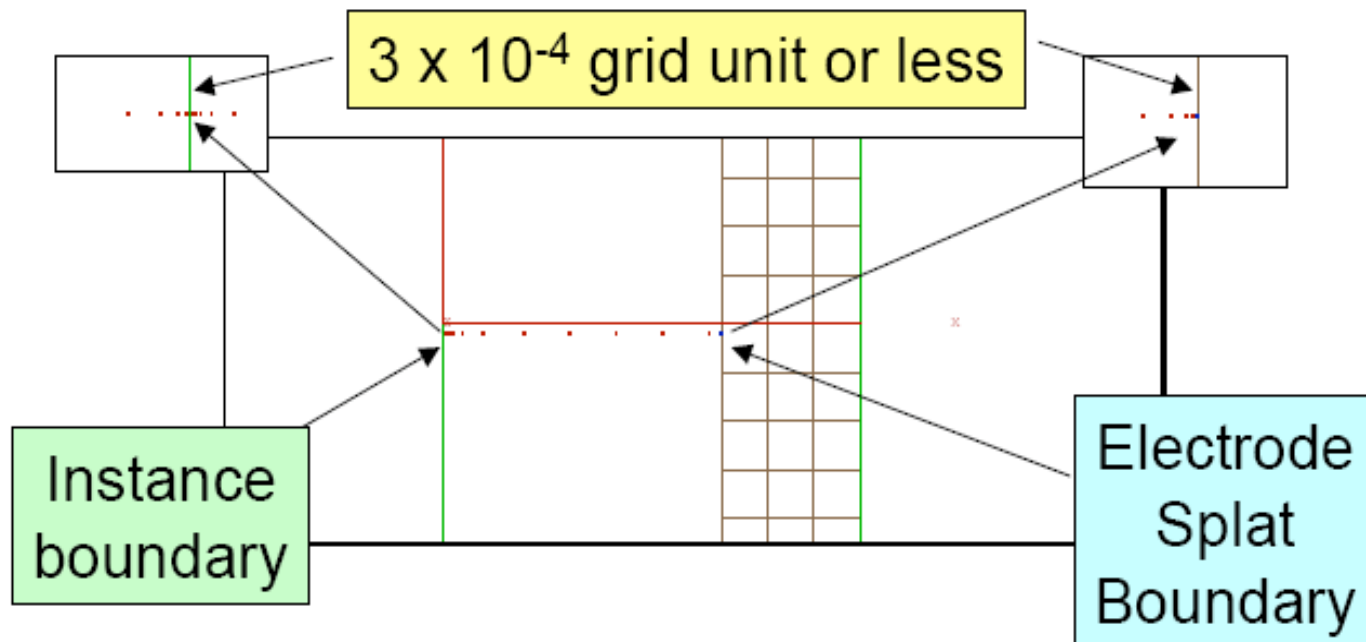
As the ion moves through the array the potential gradient is calculated at each time step for its current position, the forces are determined, and it moves based on those forces until the next time step.

Time steps can vary based on the local gradient, or can be held constant.



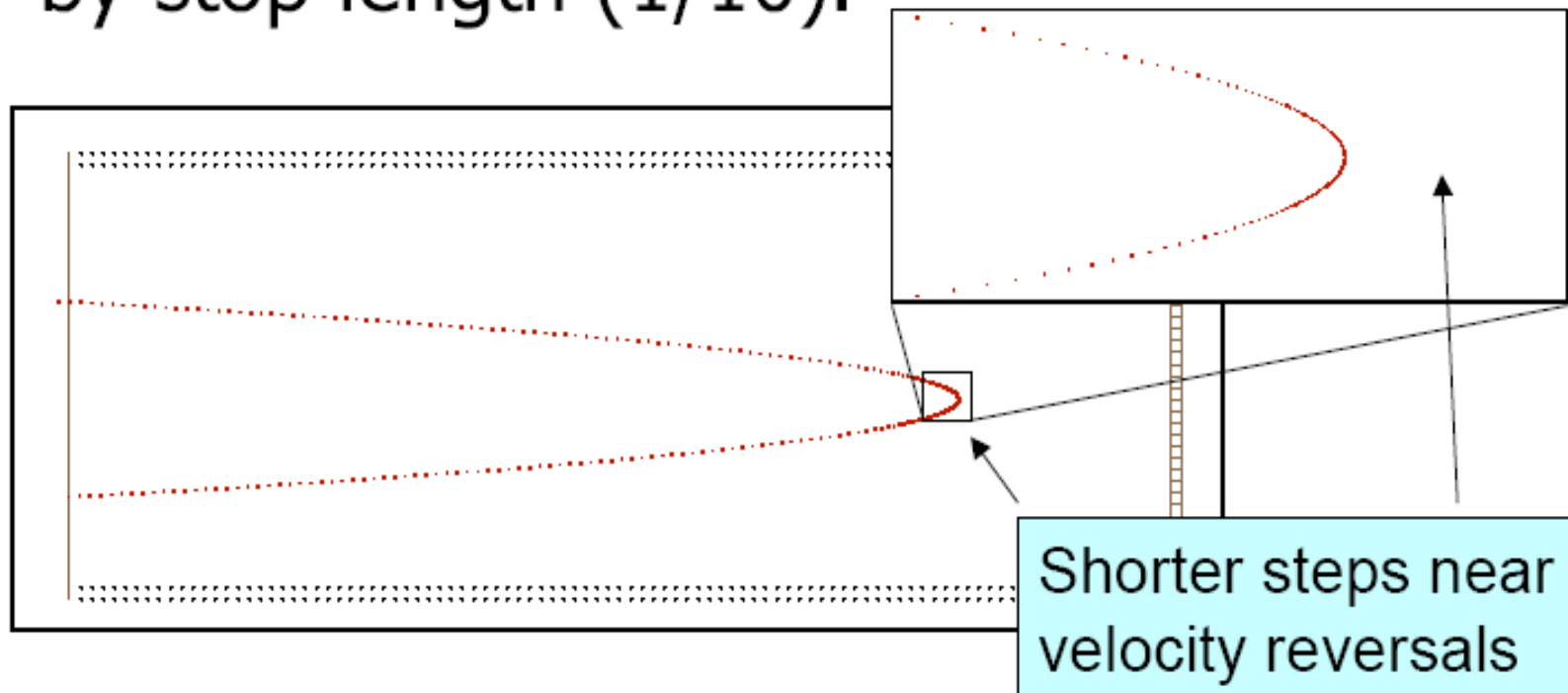
Variable Time Steps

- Detect, leap back, and halve the time step is used to approach boundaries.



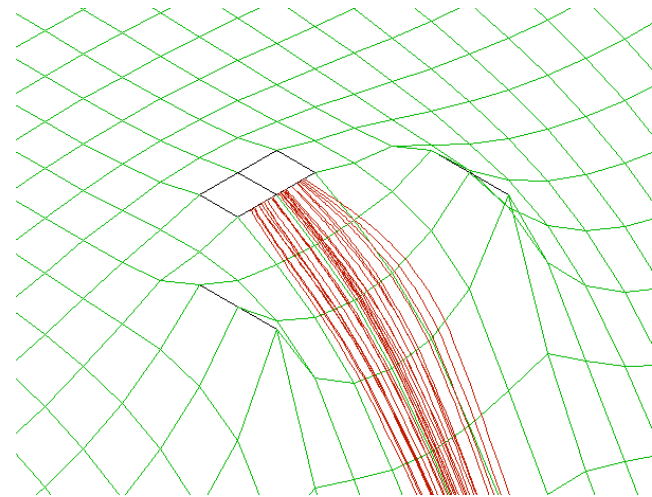
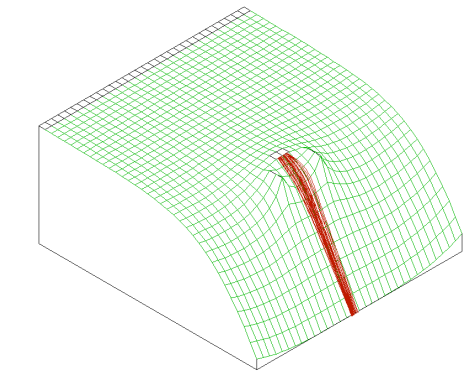
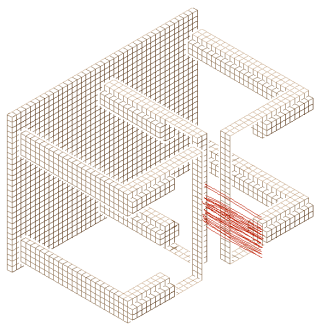
Variable Time Steps

- Fixed distance step integration is modified by stop length ($1/10$).



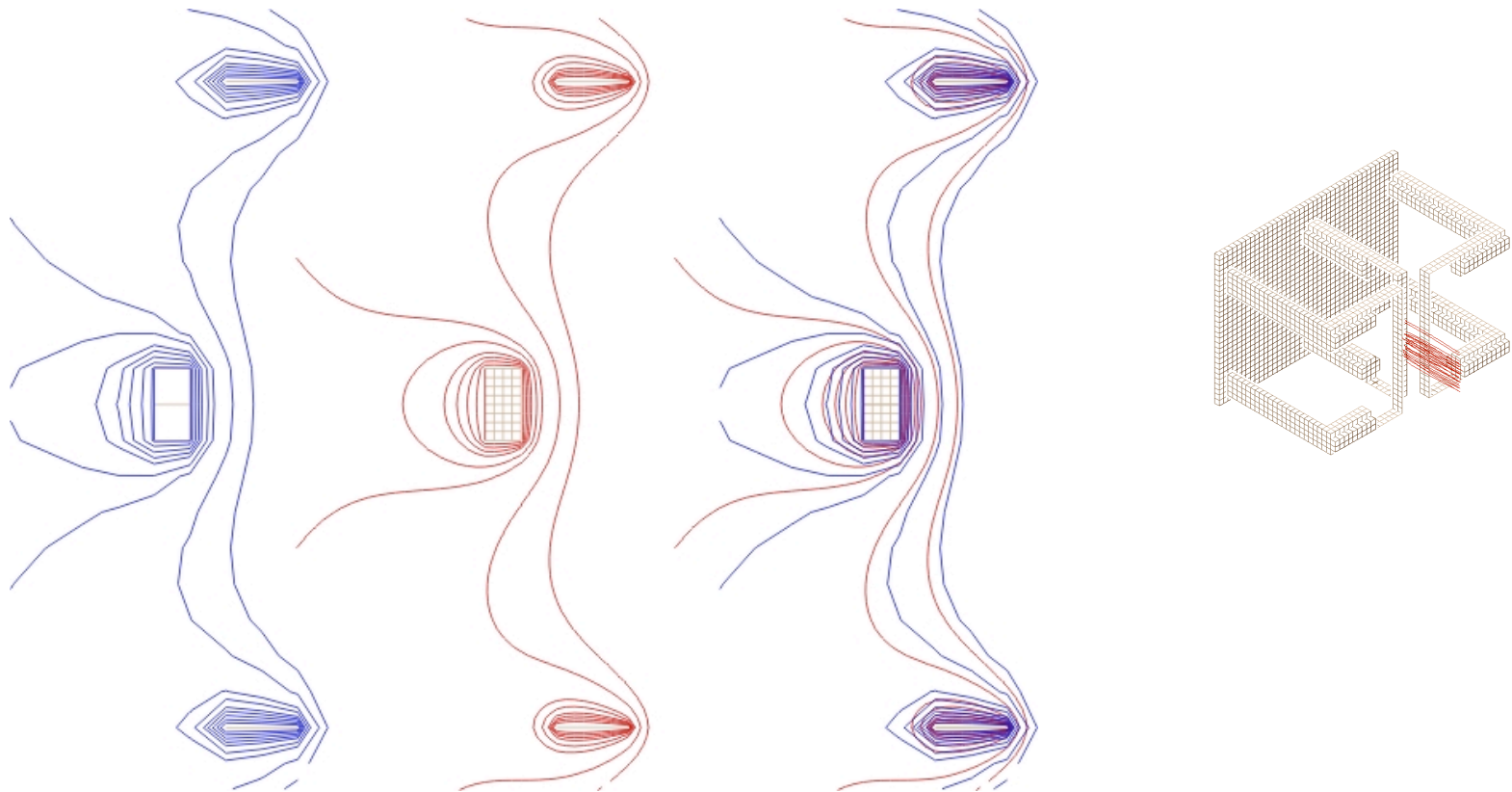
Limitations and Cautions

- Geometry definitions
 - Uniform grid
 - Spacing establishes surface “roughness”
 - Interpolation used to calculate inter-grid values
 - Near-field gradients less reliable than far-field



Limitations and Cautions

Grid density effect – quadruple resolution

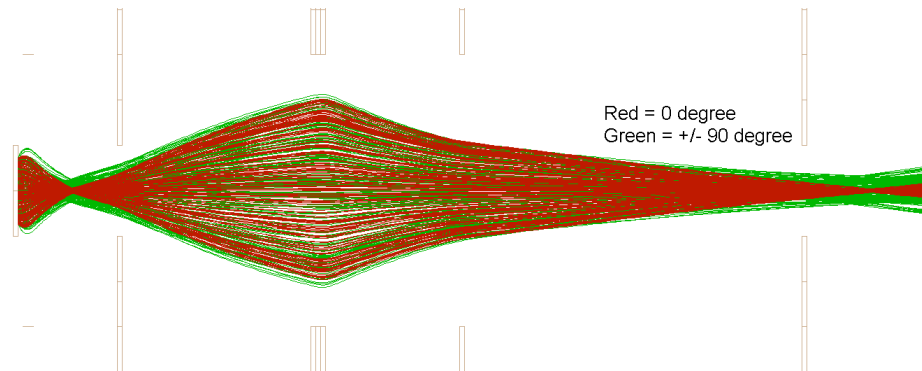


Limitations and Cautions

- Ions' initial conditions

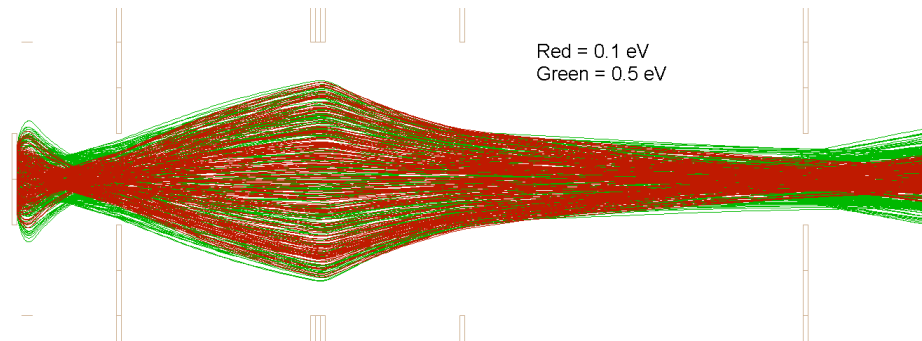
- Position

- x, y, z, angle



- Energy

- vector velocities

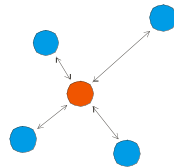


Limitations and Cautions

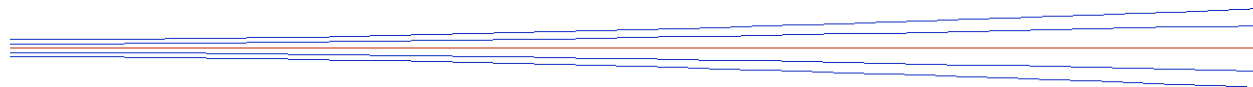
Space Charge Estimates

Two methods available to *estimate* effect of space charge on trajectories.

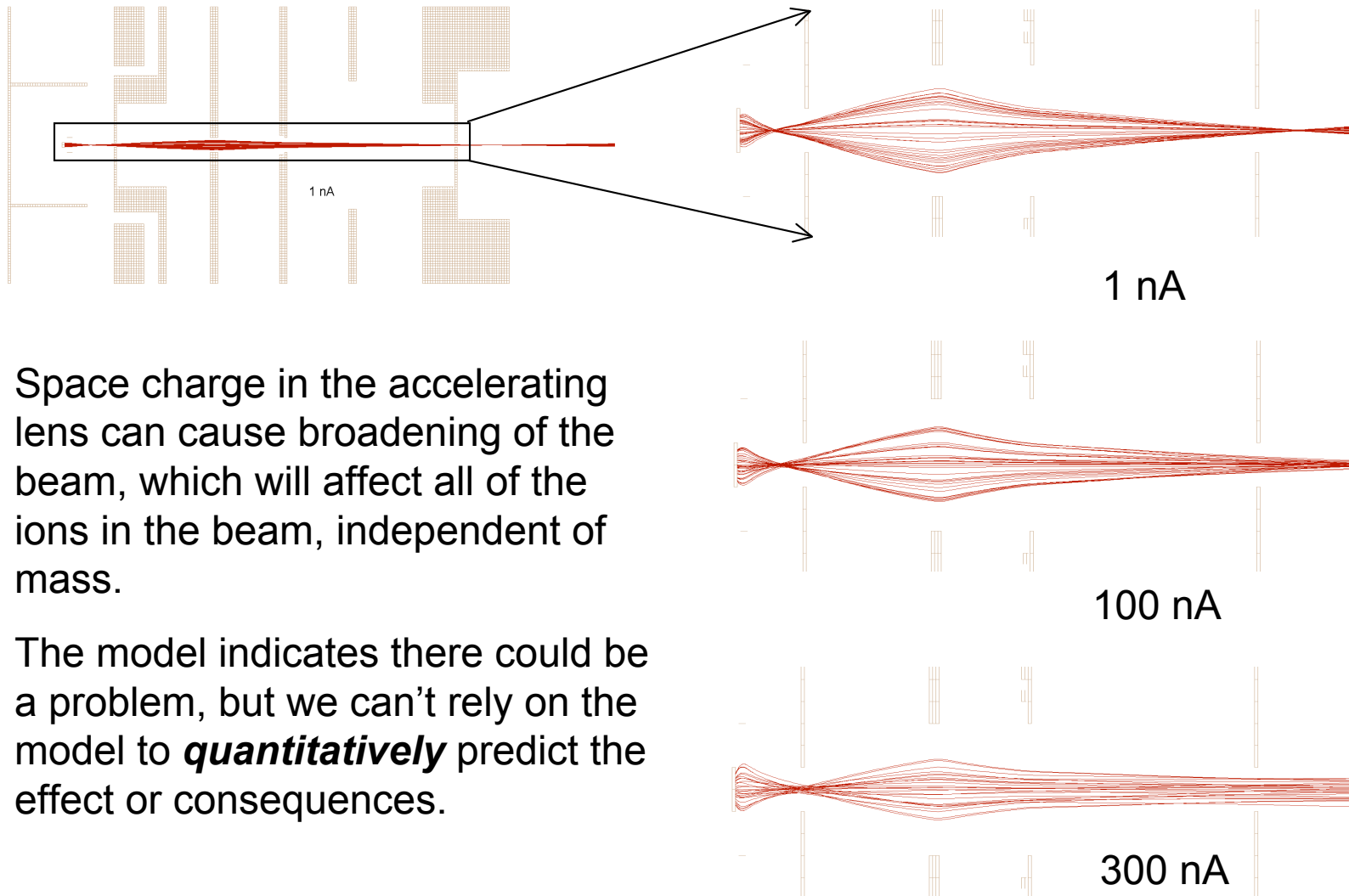
- Ion Cloud – each ion represents a small “cloud” of ions.



- Beam Repulsion – each ion represents a line charge.



Beam Space Charge Effects

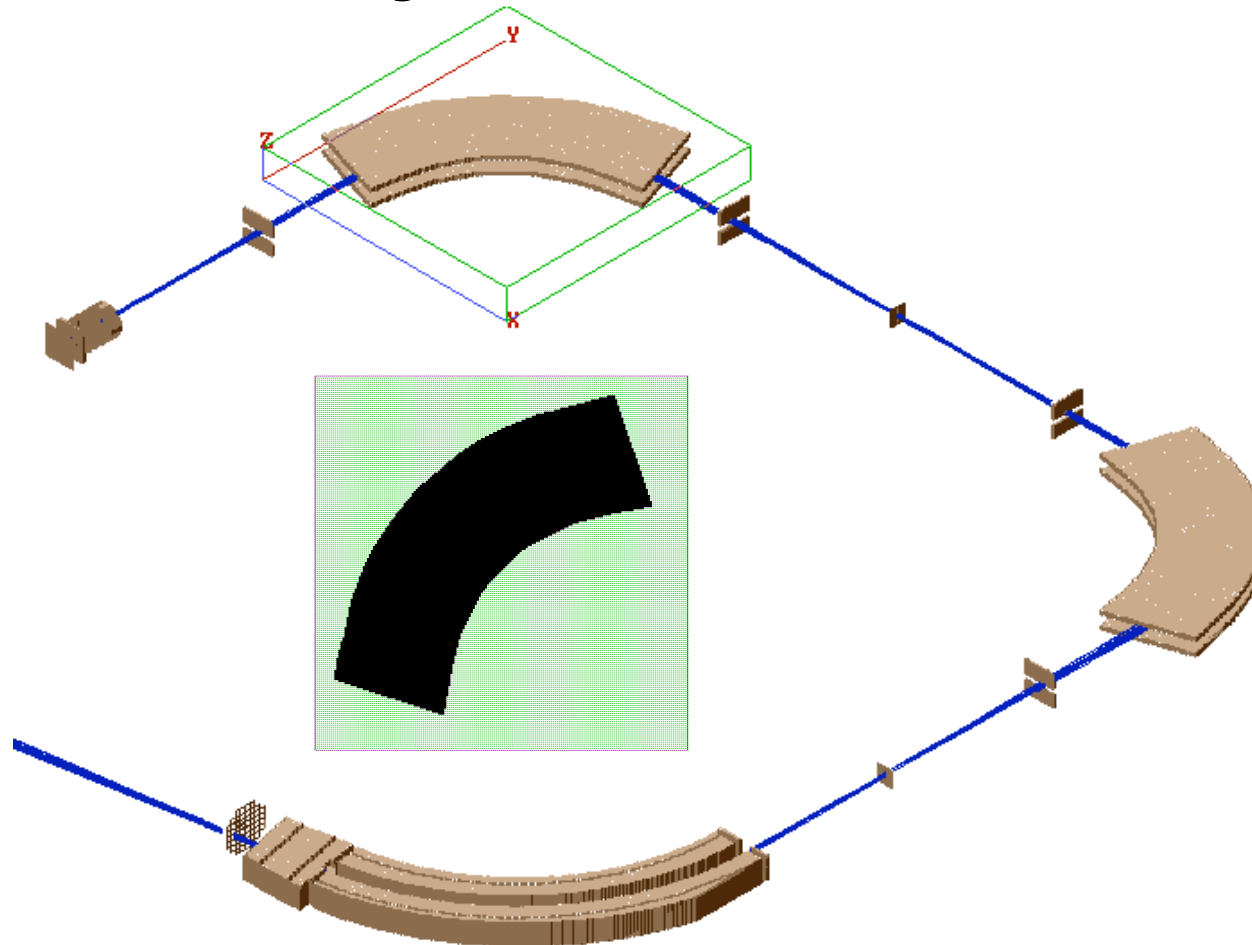


Space charge in the accelerating lens can cause broadening of the beam, which will affect all of the ions in the beam, independent of mass.

The model indicates there could be a problem, but we can't rely on the model to **quantitatively** predict the effect or consequences.

Limitations and Cautions

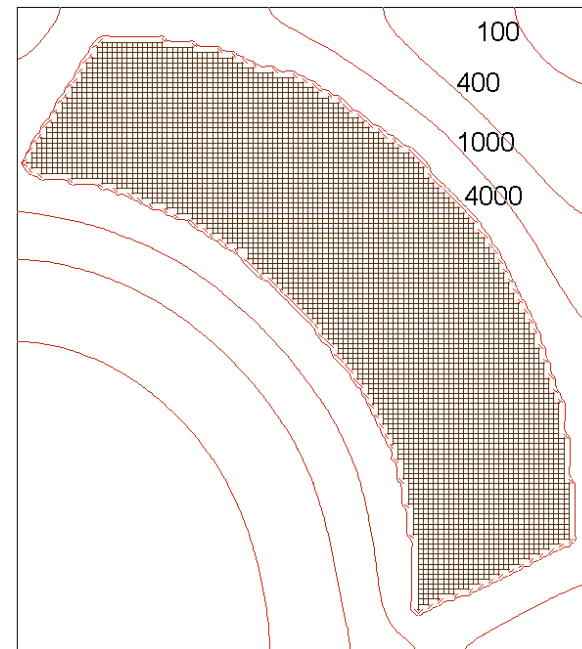
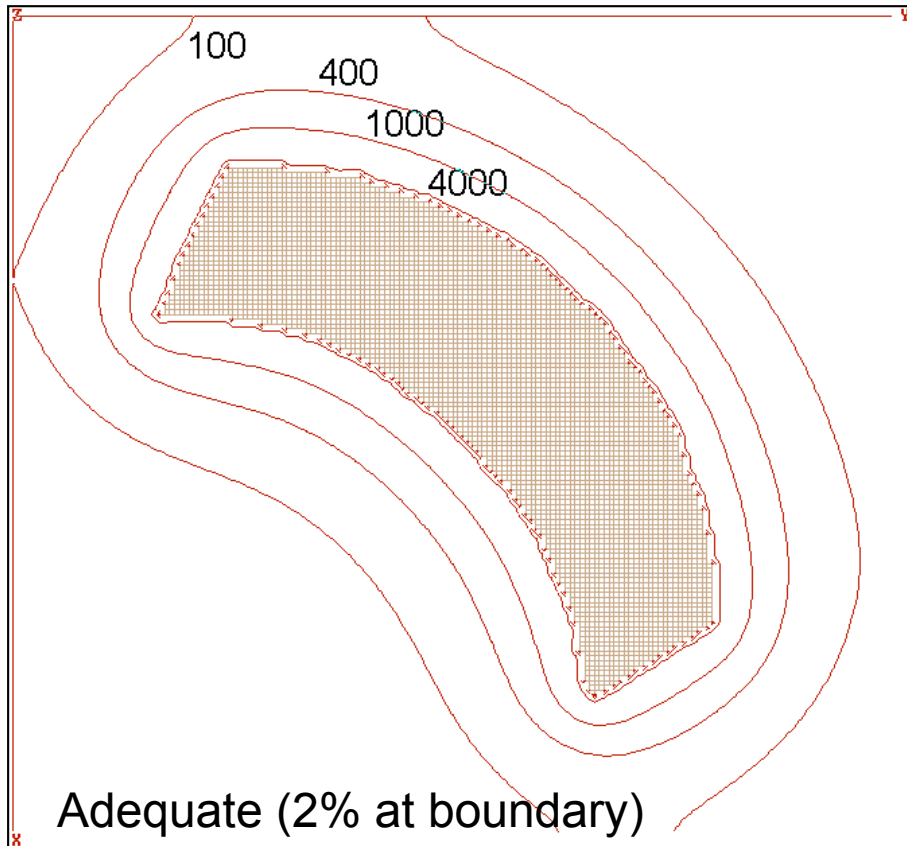
Array Boundaries



Extend array boundary far enough to prevent sharp transitions.

Limitations and Cautions

Array Boundaries



Too small

Extend array boundary far enough to prevent sharp transitions.