SIMION Beyond Ion Simulation

Field Analysis, Synthesis, and Harmonic Analysis for MS Design

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Overview

There have been some powerful changes to Simion since David Dahl's last version. Today I will mention a few that have been very useful with hope peeking your interest enough to go further.

- LUA scripting with a C API instead of PRG code
- New GEM8.2 syntax makes geometry files programable in LUA simplifies some of the more confusing methods.
- The Nelder-Mead Simplex Optimization a powerful multi-dimensional algorithm that is easy to use in LUA code when developing optimized designs.
- A generalized Poisson solver greatly extends the physics solvable in SIMION including: dielectrics, currents in resistive elements, and more.
- Adding functions, e.g GNU Scientific Library functions as DLL's
- Adding Harmonic Inversion (HARMINV) for modeling ion trajectories in traps and guides.
- Using an FFT to determine the multipole expansion of a trap.

The Generalized Poisson Solver

From Maxwell's equations we have,

$$\nabla \cdot D = \rho,$$

If $D = \varepsilon E$, then $\nabla \cdot (\varepsilon E) = \rho$, and therefore,

$$\nabla \cdot (\varepsilon \nabla \varphi) = \rho.$$

Which is the generalized Poisson's equation.

Similarly starting with conservation of charge, $\nabla \cdot J = -\frac{\partial \rho}{\partial t}$ and Ohm's Law $J = \sigma E$, we have,

$$\nabla \cdot (\sigma \nabla \varphi) = -\frac{\delta \rho}{\delta t}$$

Which the same form as the generalize Poisson's equation. Simion can now solve equations of this form.

Solving the potential is a resistive glass tube.

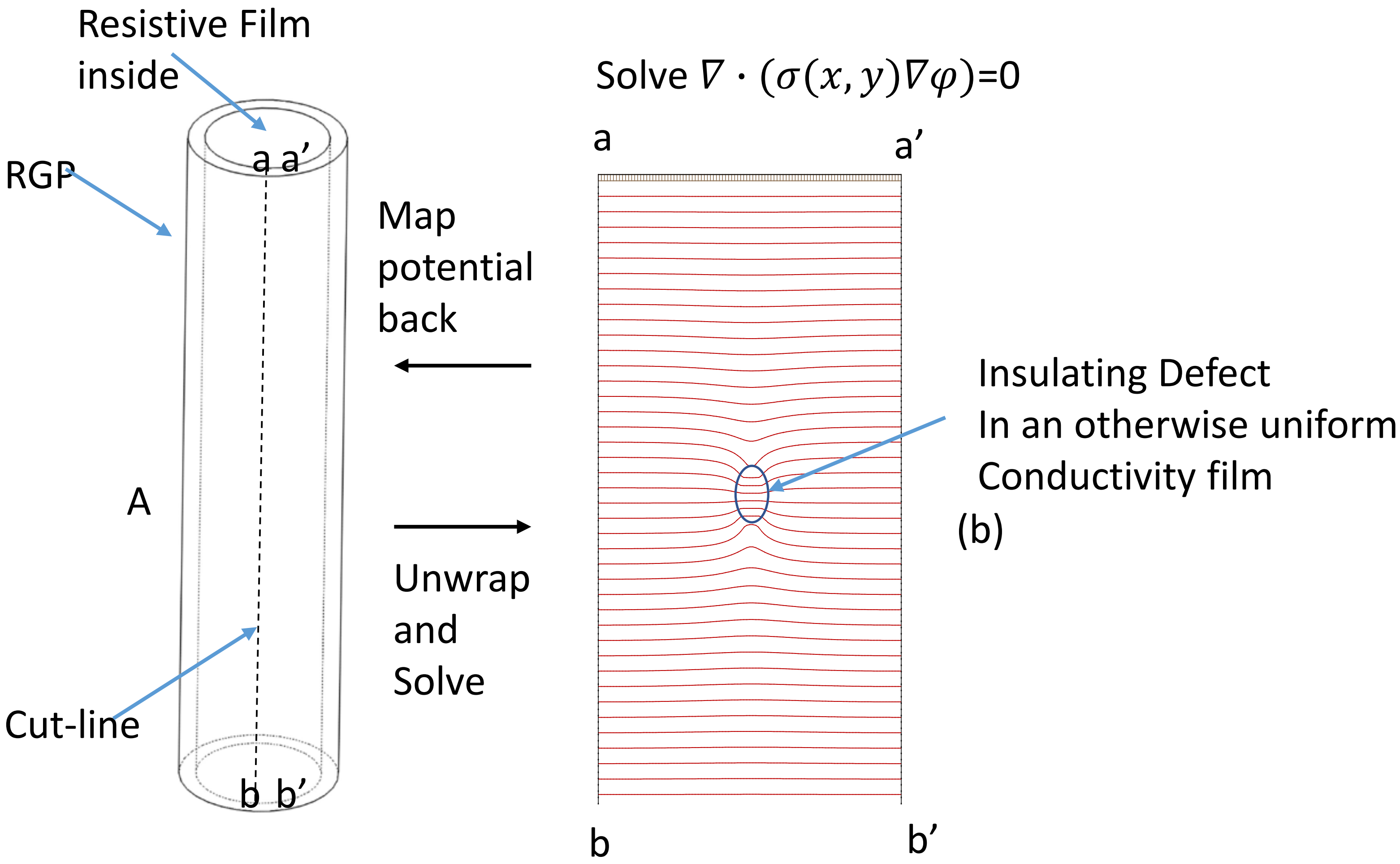


Figure 1: Scheme for mapping flat solution with periodic boundary conditions to the cylindrical resistive glass tube.
(a) Resistive glass tube showing an arbitrary cut-line for the unfolding to a flat array, (b) 2D array showing the distortion of the potential due to a small insulating defect.

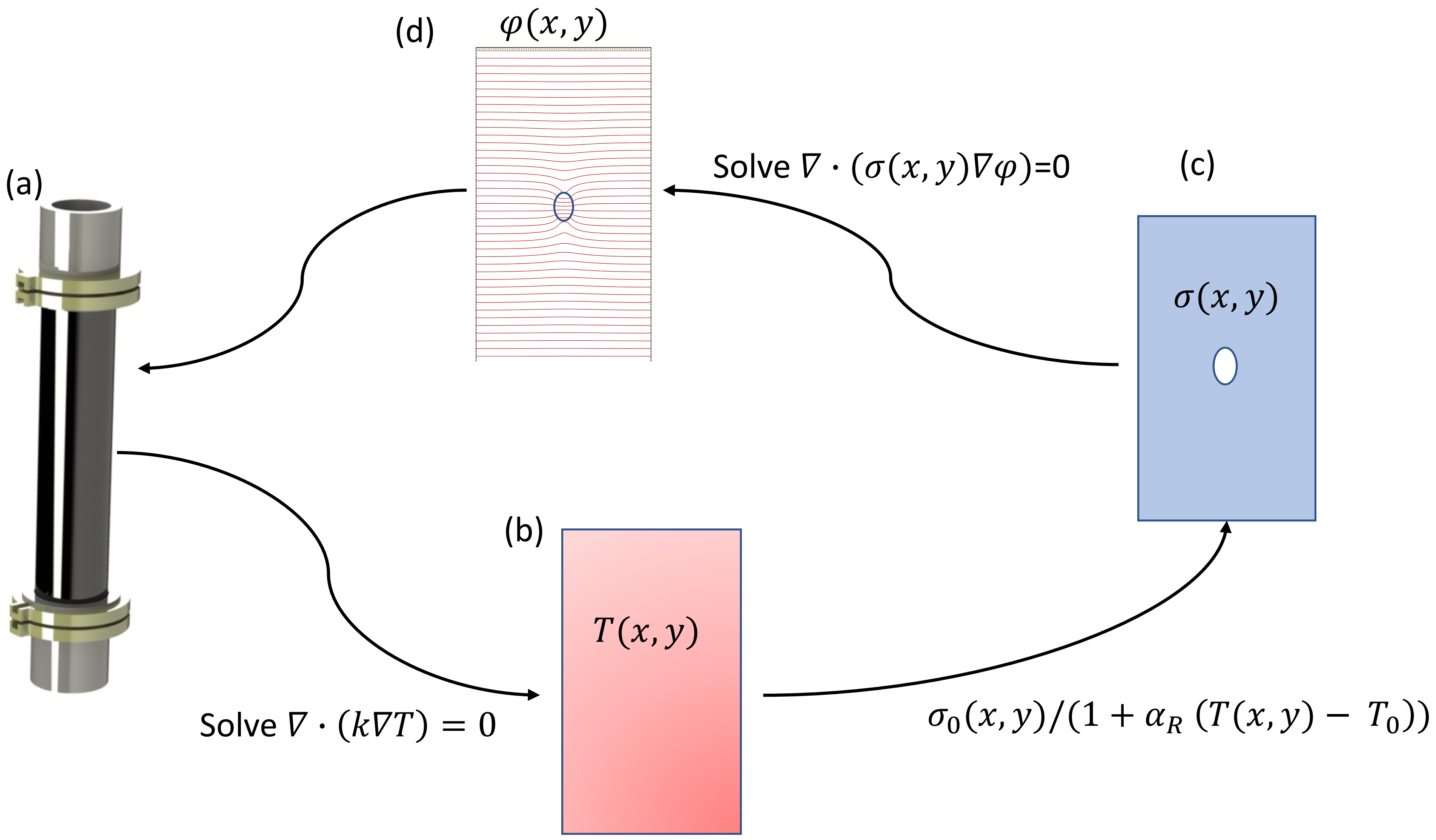


Figure 2: Overall computation cycle, (a) resistive glass assembly with inlet and outlet lenses. (b) 2D array of the film temperature, (c)2D conductivity array , 2D current density potential solution.

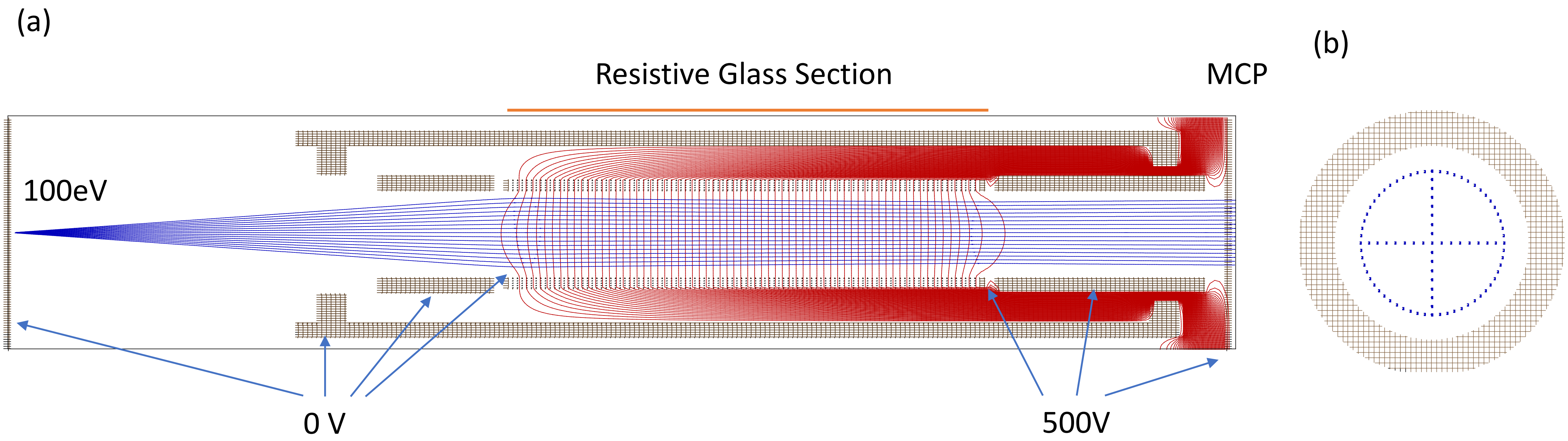


Figure 3: 3D Simulation of a uniform conductivity resistive glass cylinder. (a) contour plot and electron trajectories (b) an expanded end view of electron splats at the MCP when the beam has a cone and cross pattern with 4° half angle.

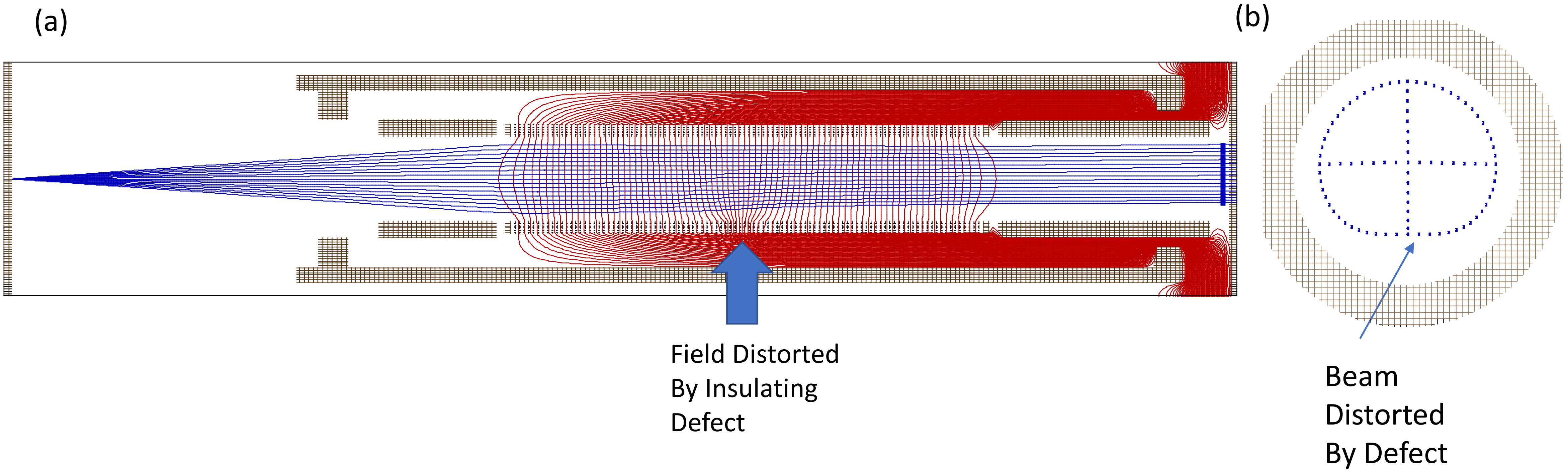


Figure 4: 3D Simulation of a uniform conductivity resistive glass cylinder with a small insulating defect. (a) contour plot and electron trajectories, (b) an expanded end view of electron splats at the MCP when the beam has a cone and cross pattern with 4° half angle showing the distortion created by the insulating defect.

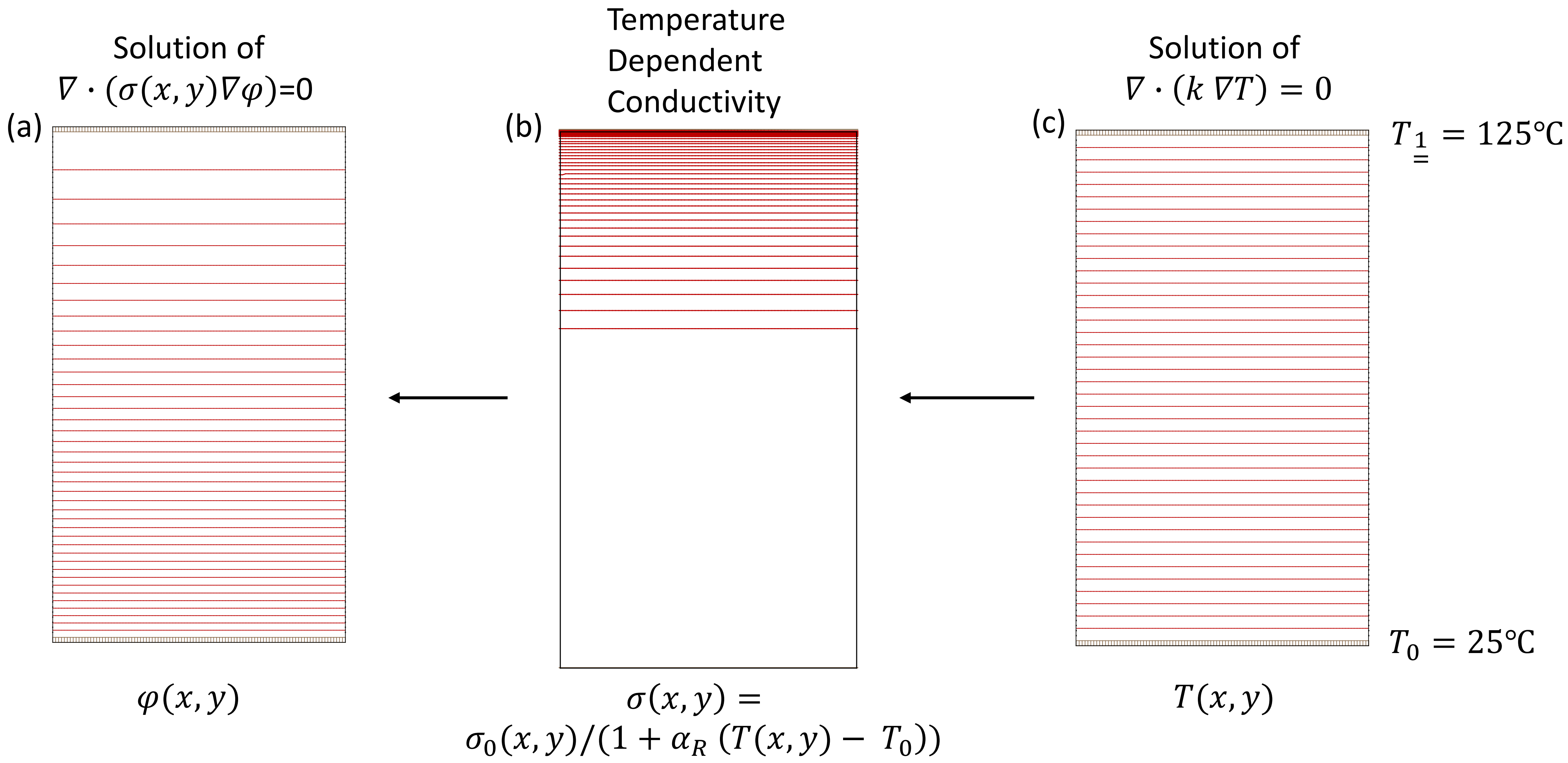


Figure 5 Calculating the potential with the conductivity varying with temperature, (a) 2D the current density potential, (b) 2D temperature dependent film conductivity , (c) linear temperature gradient due to uniform fixed end conditions.

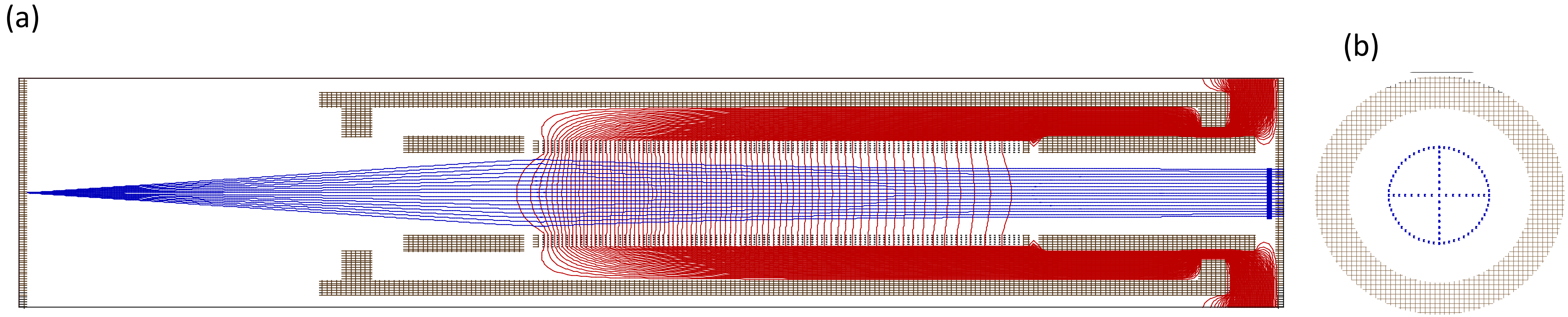


Figure 6: 3D Simulation of a uniform conductivity resistive glass cylinder with a non-uniform potential due to 100°C temperature difference, (a) contour plot and electron trajectories, (b) an expanded end view of electron splats at the MCP when the beam has a cone and cross pattern with 4° half angle showing a tighter parallel beam pattern than the uniform potential gradient.

Using Harmonic Inversion to Determine Unstable Trajectories in a Trap.

HARMINV

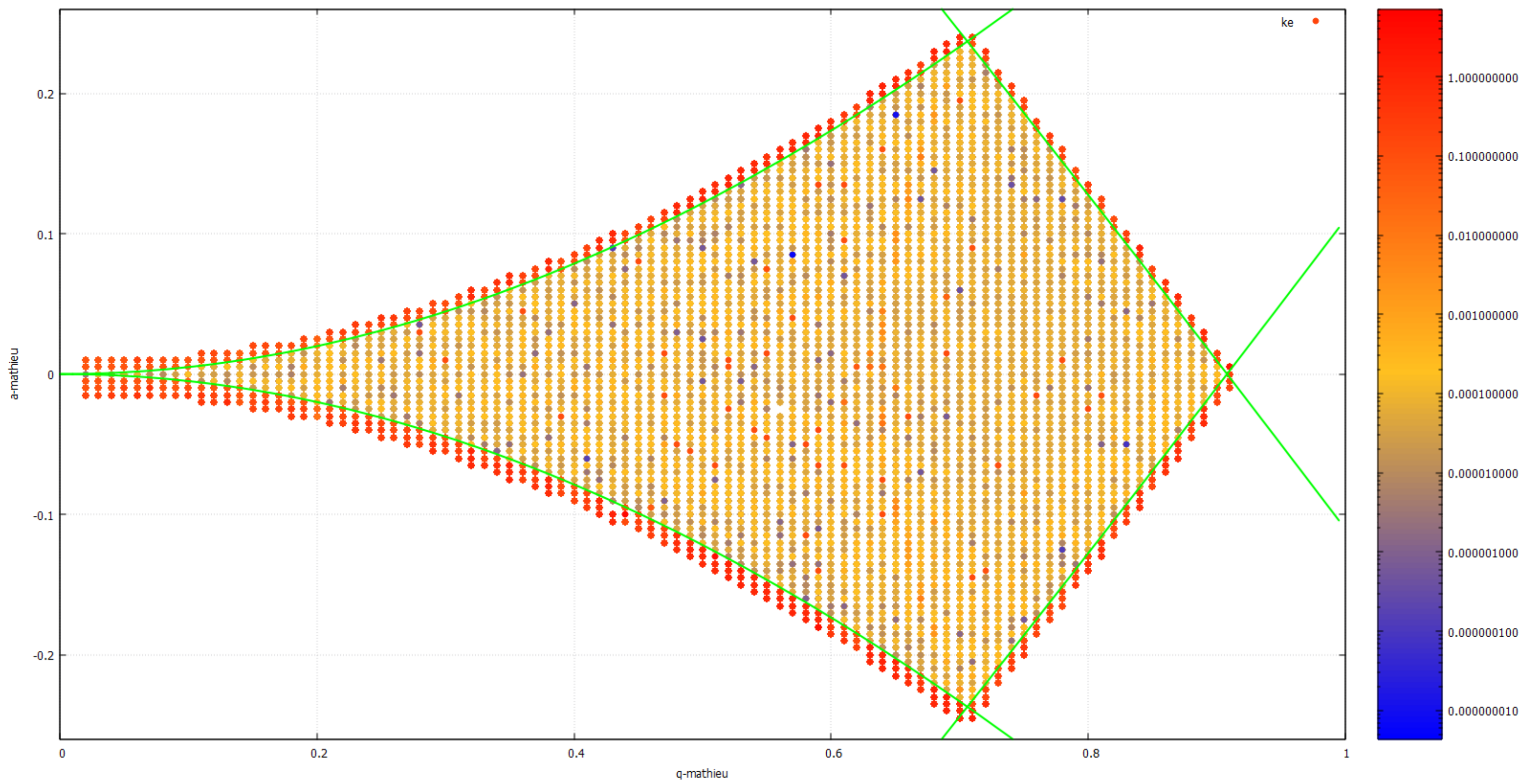
Each harmonic function fitted by HARMINV with four parameters and has the form:

$$A\, e^{-d \cdot t}\, e^{-i \cdot (2\pi \cdot f \cdot t - \varphi)} ,$$

With amplitude (A), decay constant (d), frequency (f), phase (φ), and the index (harm#). Our Simion workbench program records eight more parameters for the trajectory at our analysis point, as shown in the partial spreadsheet below.

Vrf	Vdc	qv	av	ion_ke	min	max	harm#	frequency	decay constant	Q	amplitude	phase	error
9.72E+00	0.00E+00	3.00E-02	0.00E+00	1.86E-02	0.00E+00	3.89E-02	1	-4.00E+00	4.21E-03	2.98E+03	5.58E-03	-1.63E-01	1.70E-06
9.72E+00	0.00E+00	3.00E-02	0.00E+00	1.86E-02	0.00E+00	3.89E-02	2	1.95E+00	9.22E-02	6.63E+01	1.32E-03	-8.46E-01	1.88E-04
9.72E+00	0.00E+00	3.00E-02	0.00E+00	1.86E-02	0.00E+00	3.89E-02	3	2.06E+00	2.96E-02	2.19E+02	1.26E-03	-3.27E-01	1.67E-05
9.72E+00	0.00E+00	3.00E-02	0.00E+00	1.86E-02	0.00E+00	3.89E-02	4	3.96E+00	-1.69E-04	-7.37E+04	2.34E-03	3.12E+00	4.92E-07
9.72E+00	0.00E+00	3.00E-02	0.00E+00	1.86E-02	0.00E+00	3.89E-02	5	4.00E+00	-9.20E-07	-1.37E+07	4.64E-03	-2.42E-03	2.61E-06
9.72E+00	0.00E+00	3.00E-02	0.00E+00	1.86E-02	0.00E+00	3.89E-02	6	4.04E+00	-1.08E-04	-1.18E+05	2.29E-03	-3.13E+00	4.12E-06

If we use the HARMINV data for points throughout q-a space then we can use the decay constant to show growth in trapped ions trajectory to map out a stability diagram.



Using an FFT algorithm added to Simion as a DLL, we now determine a simpler Fourier-Taylor (F-T) expansion of the potential using polar coordinates around the trapping center.

$$V(r,\theta) = \frac{V_0}{2}\sum_{n=0}^{\infty} C_n\left({}^{r}/{}_{r_0}\right)\cos(n\,\theta)$$

We analyze each potential with a fast Fourier transform of points equally space around circles of radius $0 < r/r_0 \leq 1$ centered at the trapping center, thus determining the coefficient dependence on r/r_0.

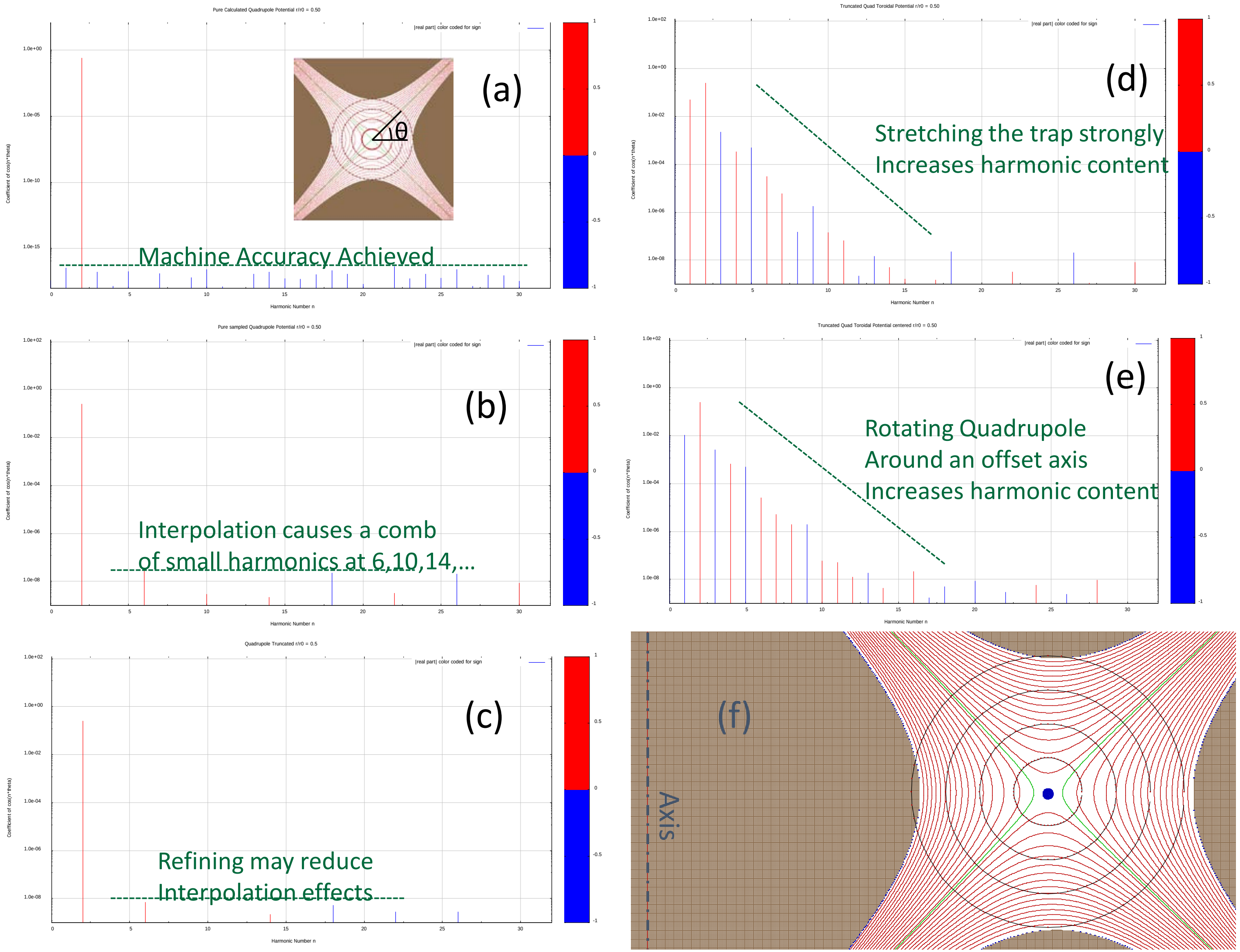


Figure 1. Potentials:(a) Calculated , (b) SIMION Interpolated, (c) Interpolated from a refined array, (d) Interpolated from stretched quadrupole trap, (e) Interpolated from toroidal quadrupole trap, and toroidal quadrupole.