Ashwood Labs

“Intrument Modeling: Simulation, Field Analysis, Synthesis, and Space-Charge

Robert Jackson
Mark Osgood

Ashwood Labs

Try Simple Geometries versus Synthesis

We used to be limited to simple machined objects, e.g cylindrical tube, round rods, *etc.*
Then we started to be able to surface machined parts from simple equations at great cost.
However, it is now reasonable to make complicated shapes with CNC machining, and even more
With additive manufacruring.

This means that if we can sythesize the fields required for and instrument,
then we can create the surfaces to create those fields. So, we need tools,
that can mathematically generate fields, parametrically optimize the performance,
create the real surfaces with truncation, slits, and possible defects, then analyze
The real field to compare to the ideal fields and possibly adjust to compensate.

To this end we will show a method to analyze the multipole components.

Fourier-Taylor Multipole analysis

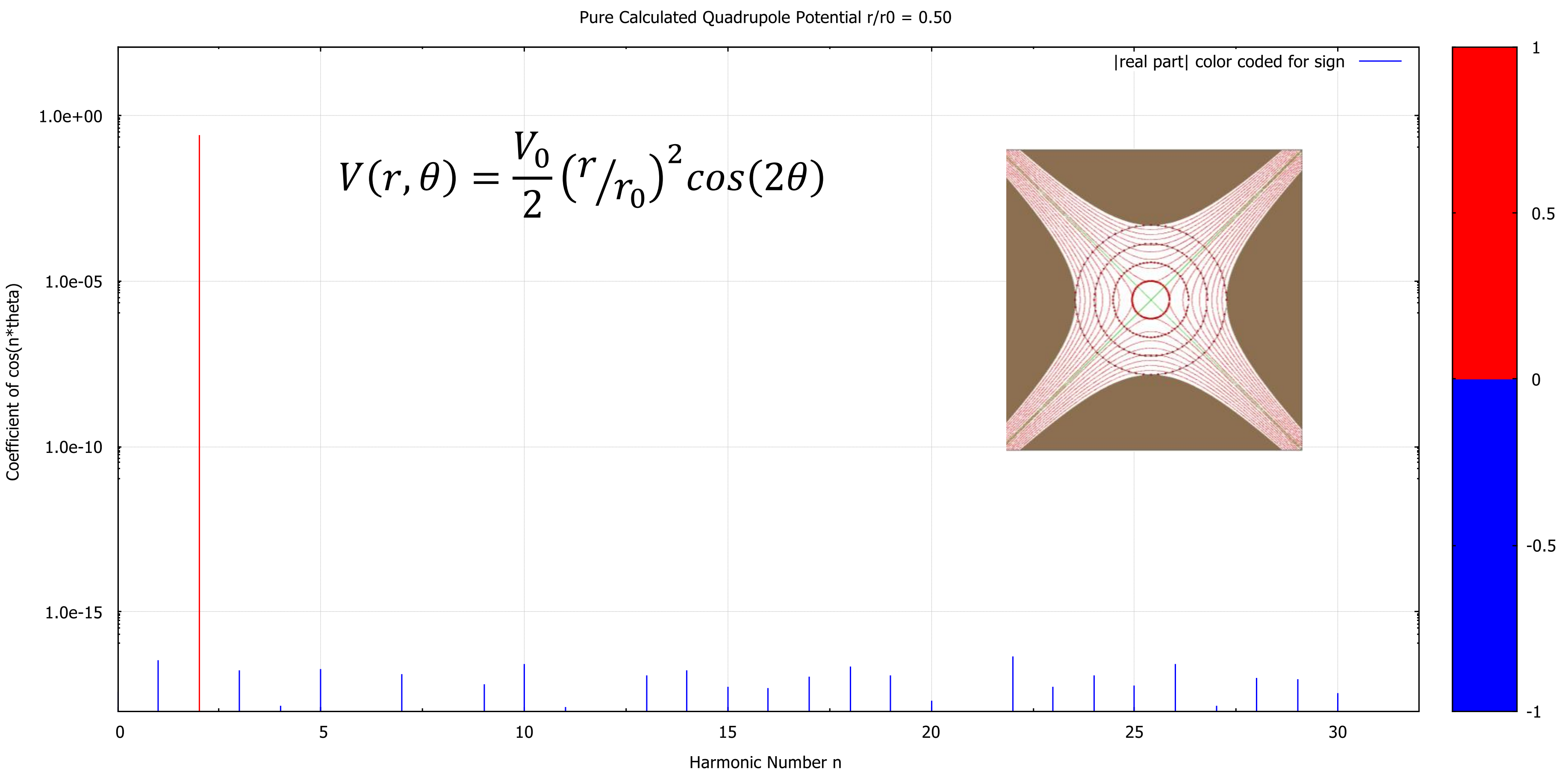
A multipole expasion about the trapping center can be written as,

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

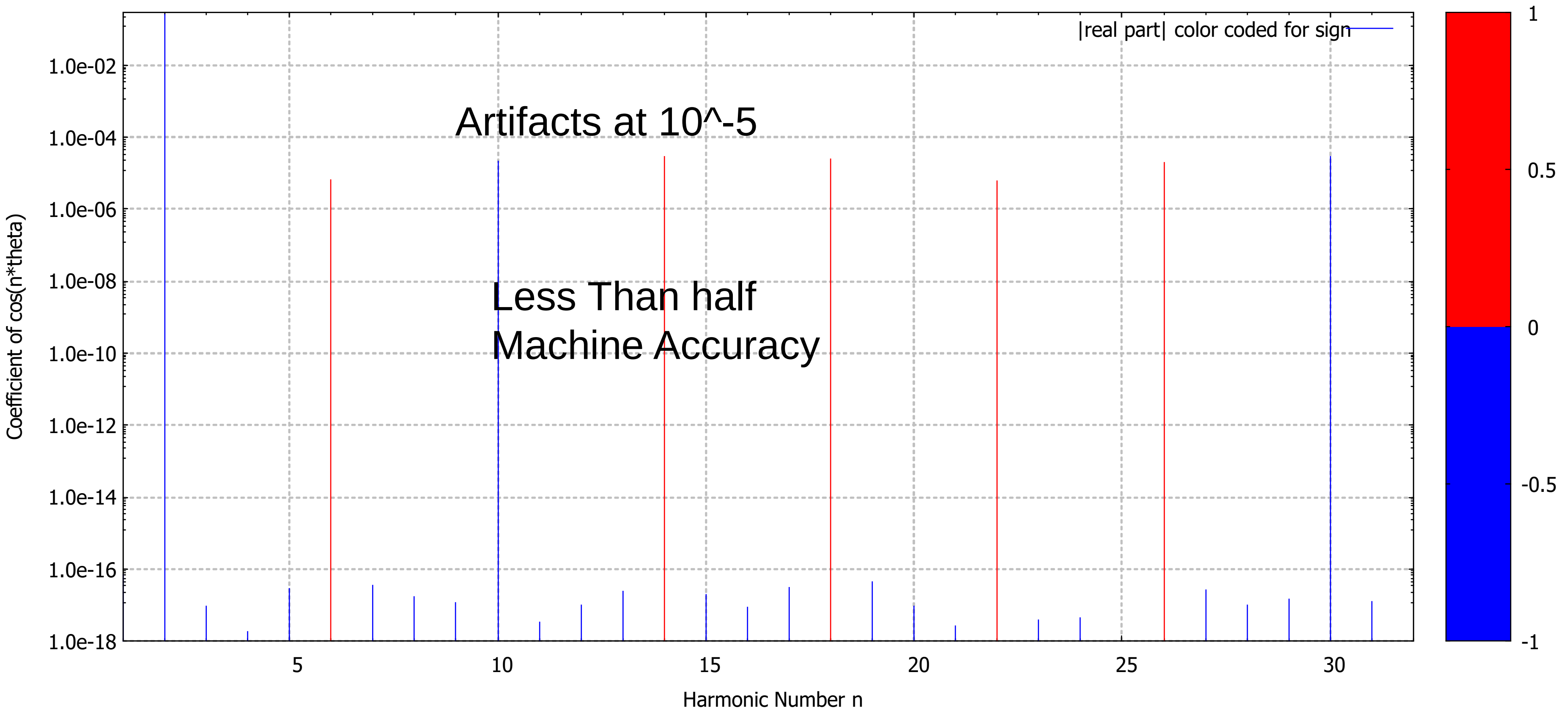
So, if we tabulate values of the potential at points evenly spaced around a circle od radius r,
then we have a Fourier cosine series and we can get the multipoile coefficients fo that radius.
This approach is easily generalized to the fourier cosine- sine series to determine rotated multipoles

Furthermore, if we do this for a series of radii then we have the coefficients as a function of ${}^{r}/_{r_0}$,
And hence we may fit a Taylor series in ${}^{r}/_{r_0}$ for each coefficient.

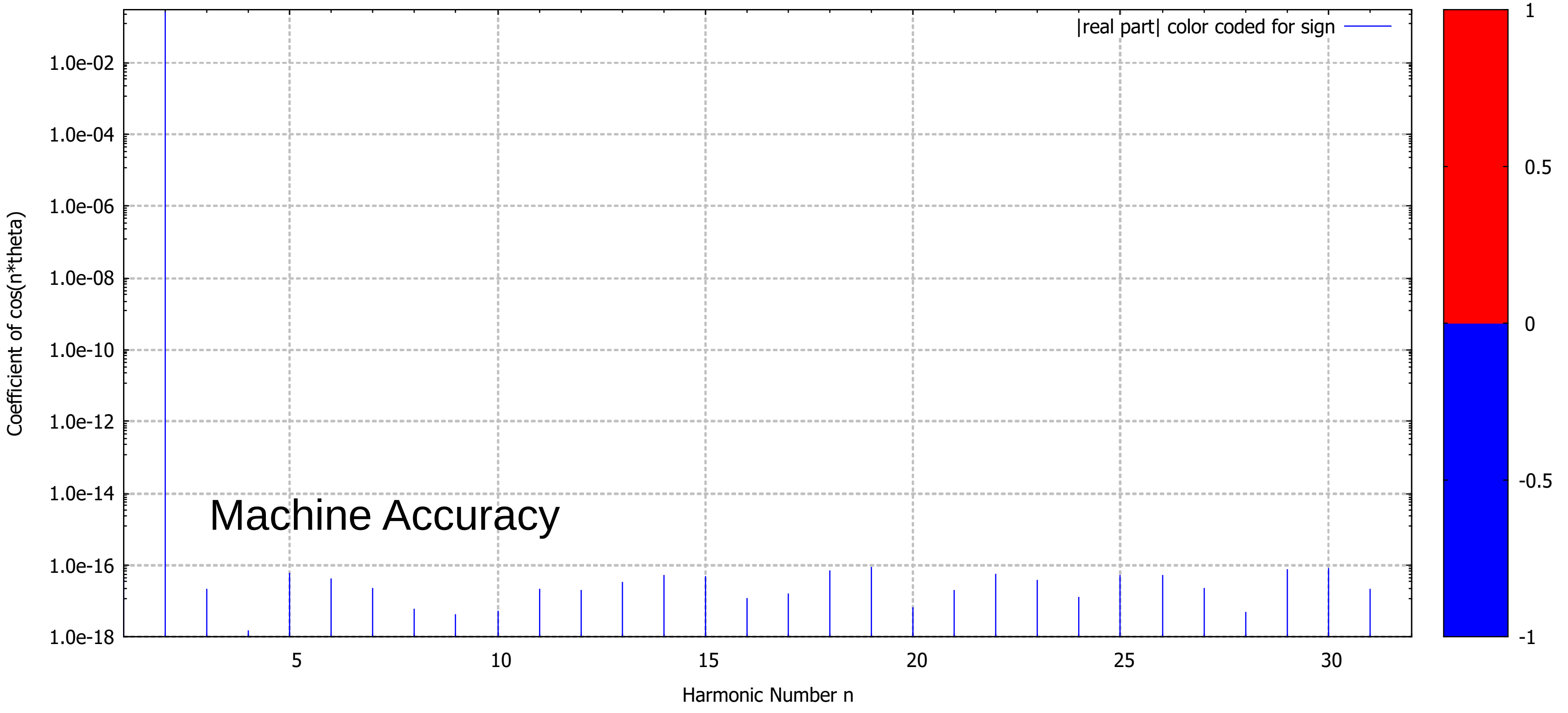
FFT Multipole analysis using an equation



FFT Multipole analysis using SIMION's bilinear interpolation of array filled from equation



FFT Multipole analysis using bicubic interpolation of array filled from equation



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.

We can also solve for the steady state temperature by $\nabla \cdot (k \nabla T) = 0$

Solving the potential in a resistive glass tube.

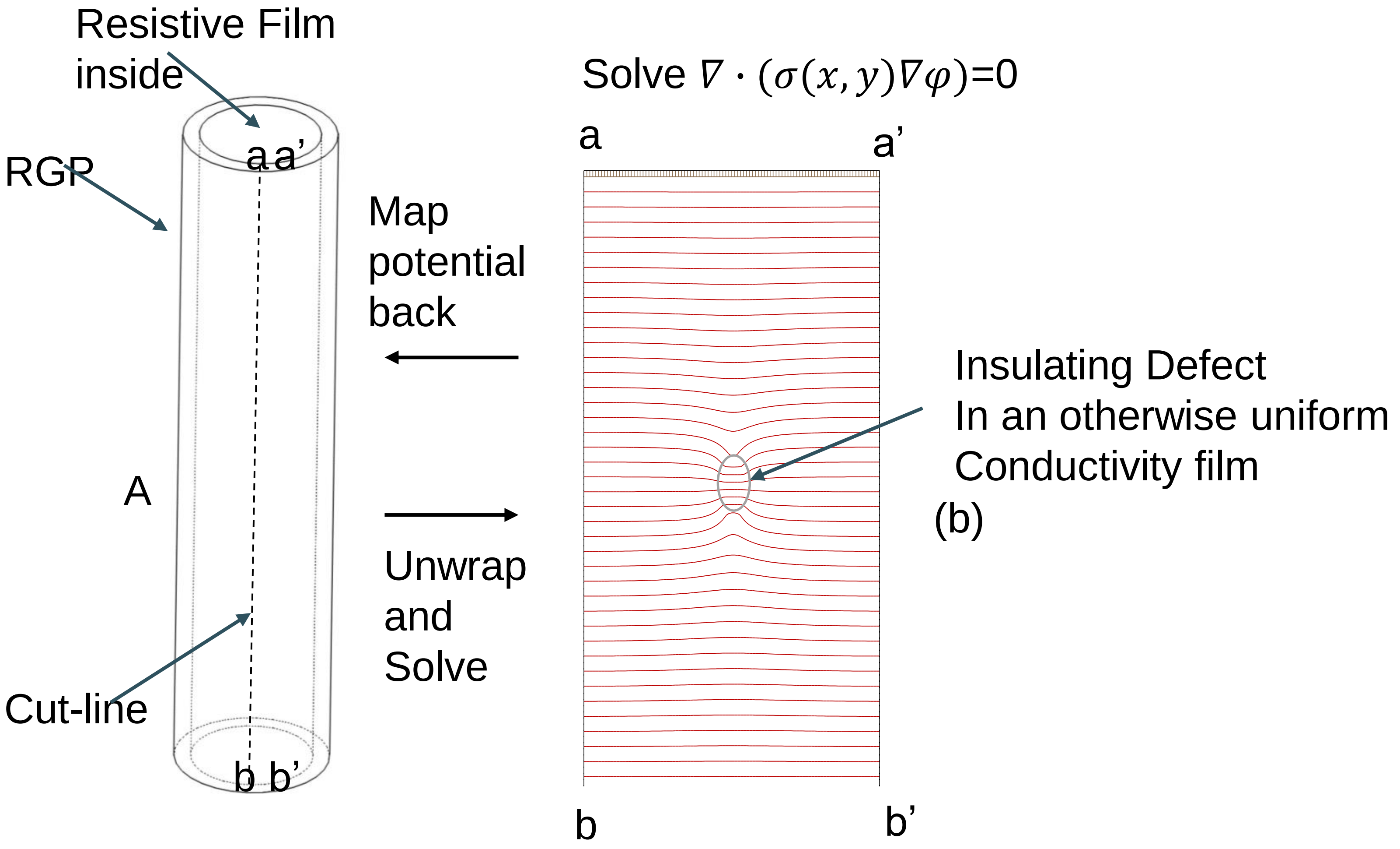
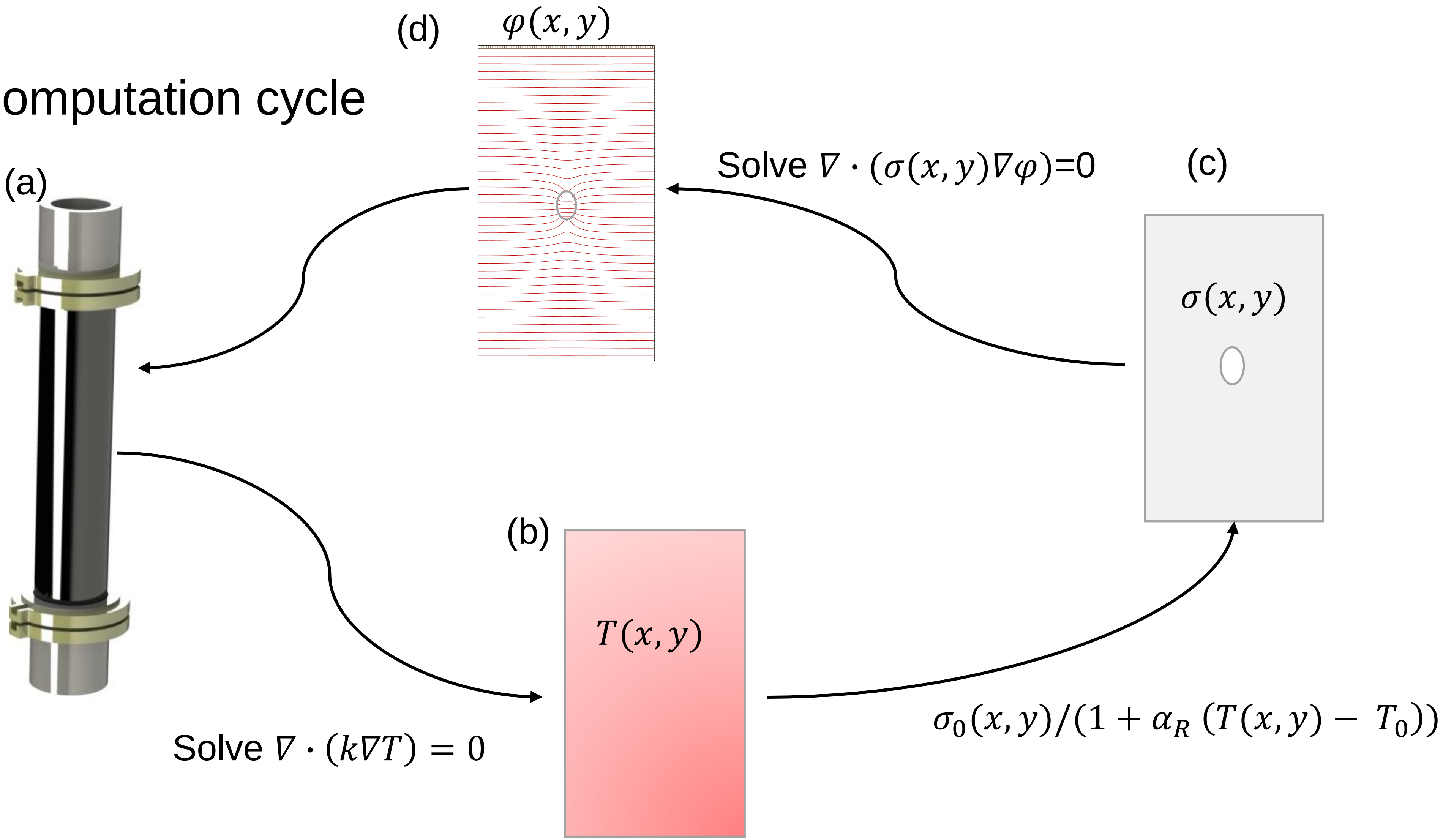


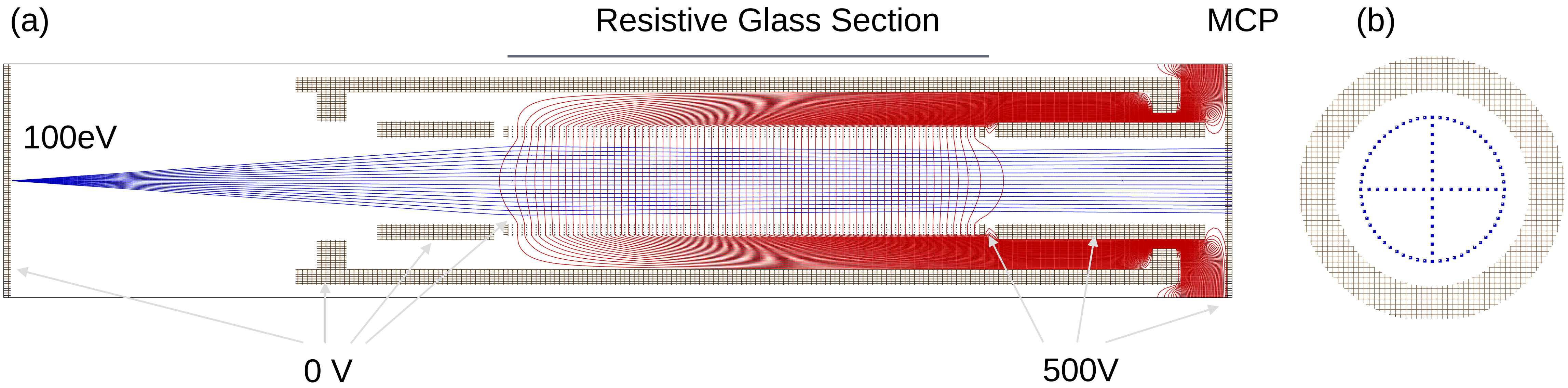
Figure 1: Scheme for mapping flat solution with periodic boundary conditions to the cylindrical resistive glass tube. Resistive glass tube showing an arbitrary cut-line for the unfolding to a flat array, (b) 2D array showing the distortion of the potential due to a small insulating defect.

Overall computation cycle



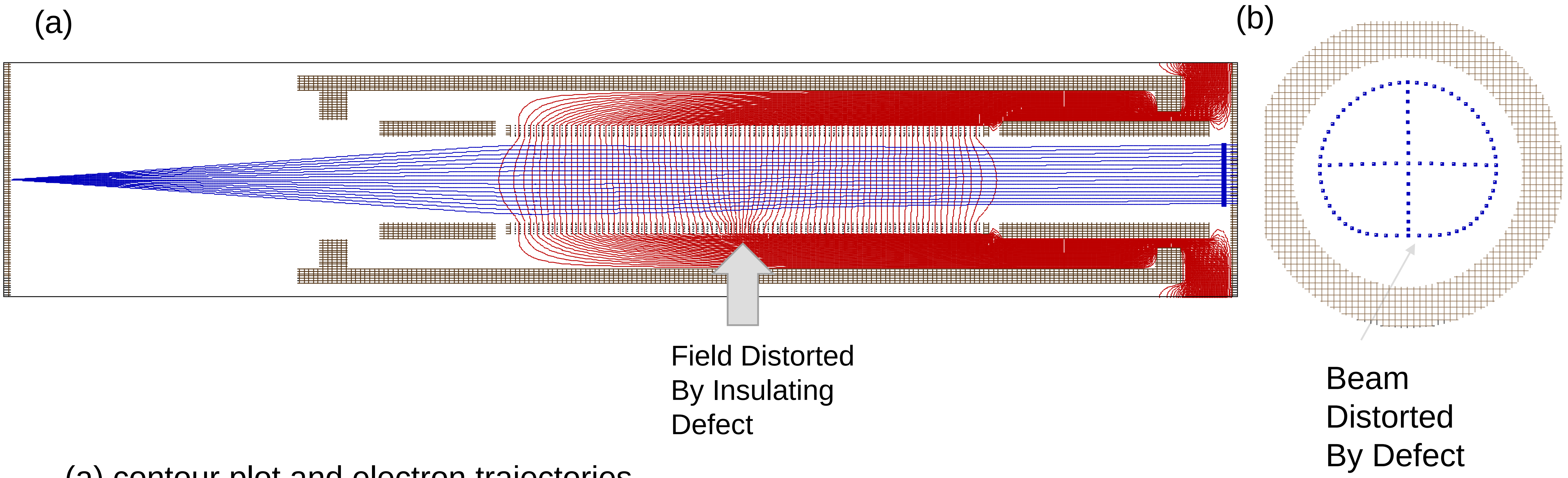
(a) resistive glass assembly with inlet and outlet lenses. (b) 2D array of the film temperature, (c)2D conductivity array , 2D current density potential solution.

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.

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.

Using Harmonic Inversion to Determine Unstable Trajectories in a Trap.

HARMINV

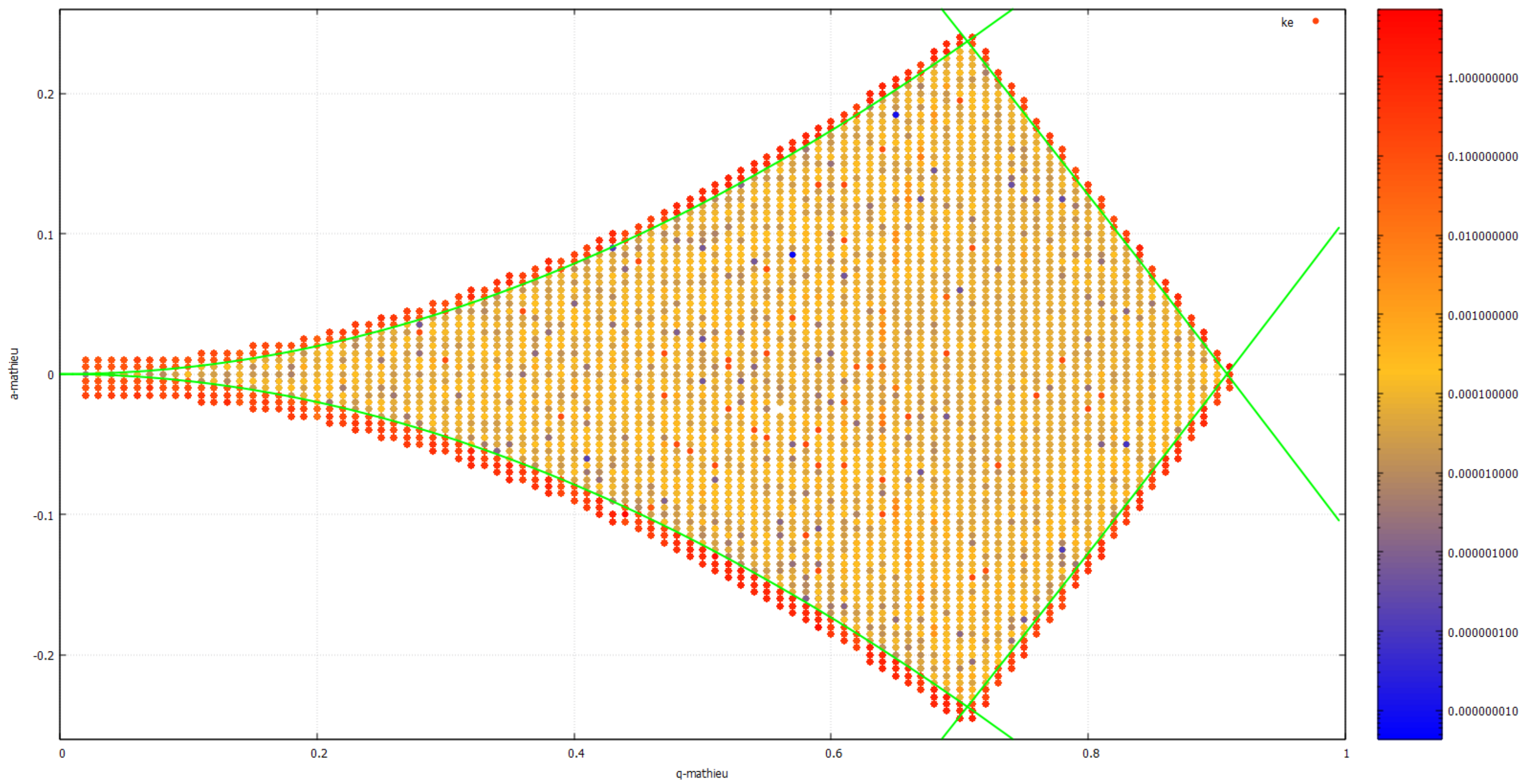
Each harmonic function fitted by HARMINV with four parameters and has the form:

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

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.

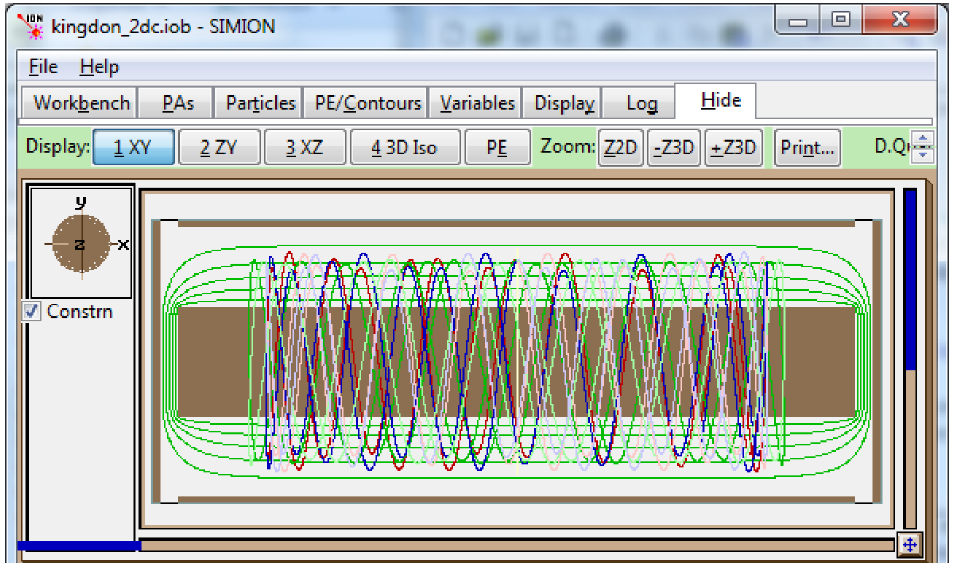
Vrf	Vdc	qv	av	ion_ke	min	max	harm#	frequency	decay constant	Q	amplitude	phase	error
9.72E+00	0.00E+00	3.00E-02	0.00E+00	1.86E-02	0.00E+00	3.89E-02	1	-4.00E+00	4.21E-03	2.98E+03	5.58E-03	-1.63E-01	1.70E-06
9.72E+00	0.00E+00	3.00E-02	0.00E+00	1.86E-02	0.00E+00	3.89E-02	2	1.95E+00	9.22E-02	6.63E+01	1.32E-03	-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

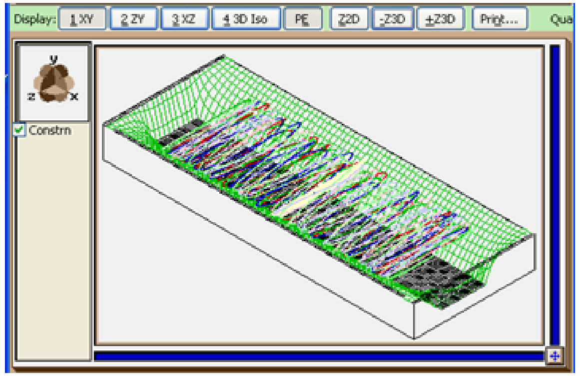
If we use the HARMINV data for points throughout q-a space then we can use the decay constant to show the onset of growth in trapped ions trajectory to map out a stability diagram. Furthermore, we can do the this as a function of initial kinetic energy of the ions to see stability near the trapping center as compared to larger orbits where the nonlinear field have more effects.



Solving for space charge in ion traps

1) Electrostatic traps, e.g. The Kingdon trap.





We can now use the generalized Poisson solver to Solve,

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

Q: But how do we get the space charge ρ?
A:Start with a guess and use ion trajectories to estimate the space charge, resolve and fly again,… continue to self consistency.

A "current mode" simulation whereby a test charge is emmited from a source and we consider the path to be a path of current through the space so that we can record that currents charge density. If we carefully choose a realistic collection of test charges, we can have reasonable estimate of ρ after several interations.

Even this method can take a great deal of computation for a trap.

Ashwood Labs

Latest Generation GPUs

>1TFLOP FP64 (Double Precision) on your desk

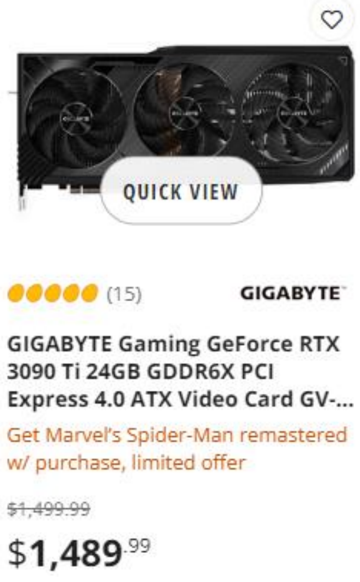
Enabling Deep Simulation at low cost

Graphics Card	RTX 3090 FE Founders Edition
GPU Codename	GA102
GPU Architecture	NVIDIA Ampere
GPCs	7
TPCs	41
SMs	82
CUDA Cores / SM	128
CUDA Cores / GPU	10496
Tensor Cores / SM	4 (3rd Gen)
Tensor Cores / GPU	328 (3rd Gen)
RT Cores	82 (2nd Gen)
GPU Boost Clock (MHz)	1695
Peak FP32 TFLOPS (non-Tensor)[1]	35.6

…API: CUDA, OpenCL, HIP, etc
…Framework: Tensor Flow, PyTorch, etc

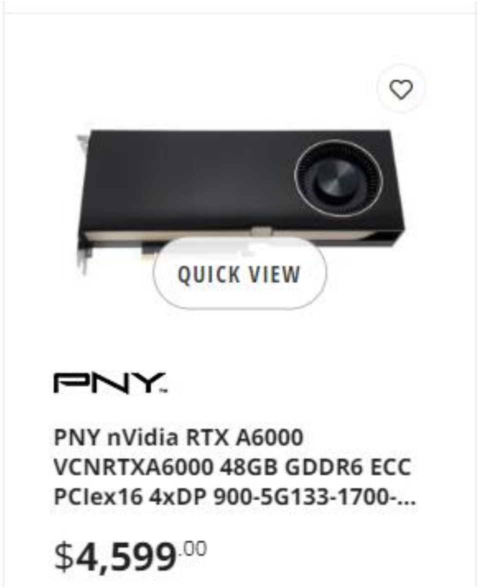
NVIDIA GA10X Ampere Architecture

Consumer Grade



FP64 (double) performance: 625.0 GFLOPS (1:64)

Workstation Grade



FP64 (double) performance: 1,210 GFLOPS (1:32)

Ashwood Labs

Additive Fabrication Technologies

Enable New Design Paradigm

FDM (Fused Deposition Modelling)

-Metal: BASF Ultrafuse 316L Metal 3D Printing

SLA (Stereo Lithography)

SLS (Selective Laser Sintering)

MJF (Multijet Fusion)

DMLS (Direct Metal Laser Sintering)

3D Printed Lost Wax Casting

…

- Rapid Prototyping
- Generative Design
- Un-machinable Trapped Geometries
- etc…