Simulation activities at SINP: an update

Supratik Mukhopadhyay

ANP Division, Saha Institute of Nuclear Physics

on behalf of the SINP group

Outline

- Background
- Recent developments
- Applications
- On-going work
- Future plan (experiments!)

Members (alphabetical order):

- Purba Bhattacharya
- Sudeb Bhattacharya
- Nayana Majumdar
- Supratik Mukhopadhyay

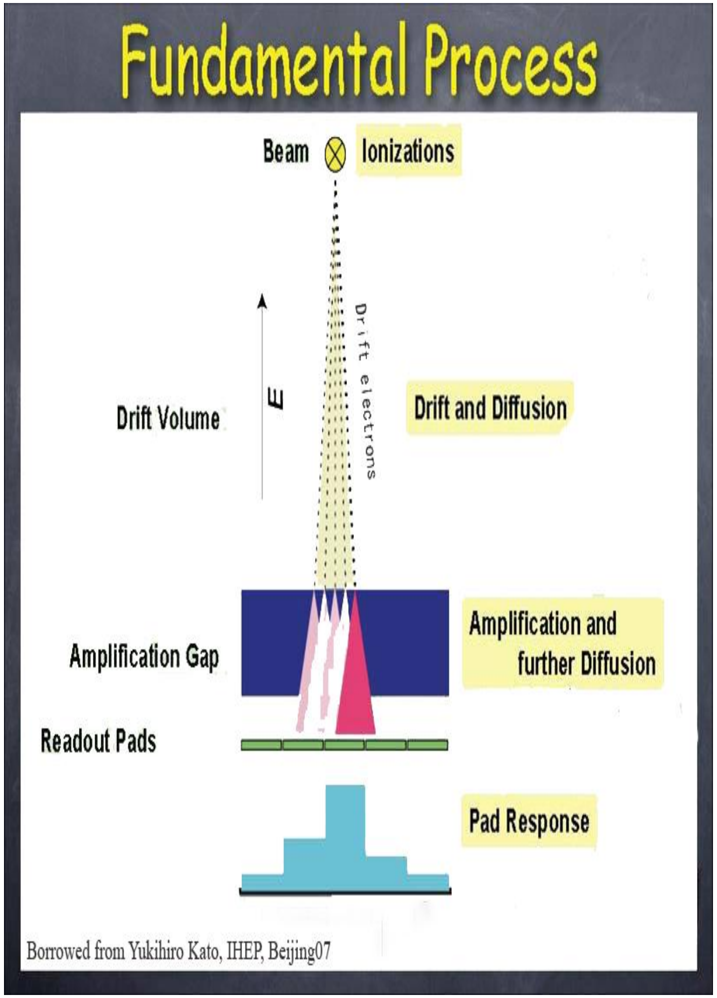
Both experimental and numerical simulation activities being carried out at SINP. At present, we are in a developmental phase, setting up the laboratory, building devices and improving the solver.

Background

Detector Simulation and neBEM

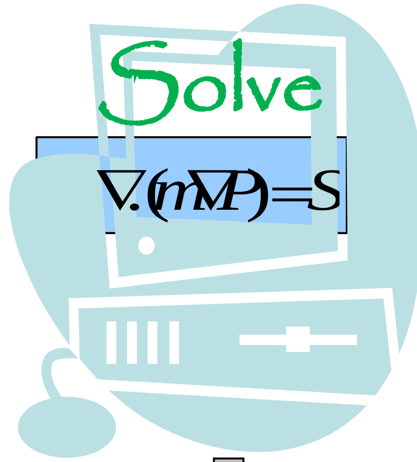
Nuclear detector simulation

How to proceed?



- Field Solver – commercial FEM packages (e.g., **MAXWELL**)
- Particle interaction to charge induction – **Garfield** framework
  - **Ionization:** energy loss through ionization of a particle crossing the gas and production of clusters - **HEED**
  - **Drift and Diffusion:** electron drift velocity and the longitudinal and transverse diffusion coefficients - **MAGBOLTZ**
  - **Amplification:** Townsend and attachment coefficients - **IMONTE**
  - **Charge induction**:involves application of Reciprocity theorem (Shockley-Ramo's theorem), Particle drift, charge sharing (pad response function - PRF) - **GARFIELD**
- Signal generation and acquisition - **SPICE**

The Field Solver is crucial at every stage – Poisson equation



BEM

- ✓ Reduced dimension
- ✓ Accurate for both potential and its gradient
- ✓ Simpler surface mesh

- x Complex numerics
- x Numerical boundary layer
- x Numerical and physical singularities

Analytic

- ✓ Exact
- ✓ Simple Interpretation

- × Restricted
- x 2D geometry
- x Small set of geometries

FEM / FDM

- ✓ Nearly arbitrary geometry
- ✓ Flexible

- x Complex volume mesh
- x Solves for potential
- x Interpolation for non-nodal points
- x Field values liable to be inaccurate (often by 50% or more!
- x Field variation jagged instead of being smooth
- x Difficulty in unbounded domains

BEM Basics

Green's identities → Boundary Integral Equations

Potential *u* at any point *y* in the domain *V* enclosed by a surface *S* is given by

$$u(y) = \int_S U(x,y)q(x)dS(x) - \int_S Q(x,y)u(x)dS(x) + \int_V U(x,y)b(x)dV(x)$$

where *y* is in *V*, *u* is the potential function, $q = u_{,n}$, the normal derivative of *u* on the boundary, *b(x)* is the body source, *y* is the load point and *x*, the field point. *U* and *Q* are fundamental solutions

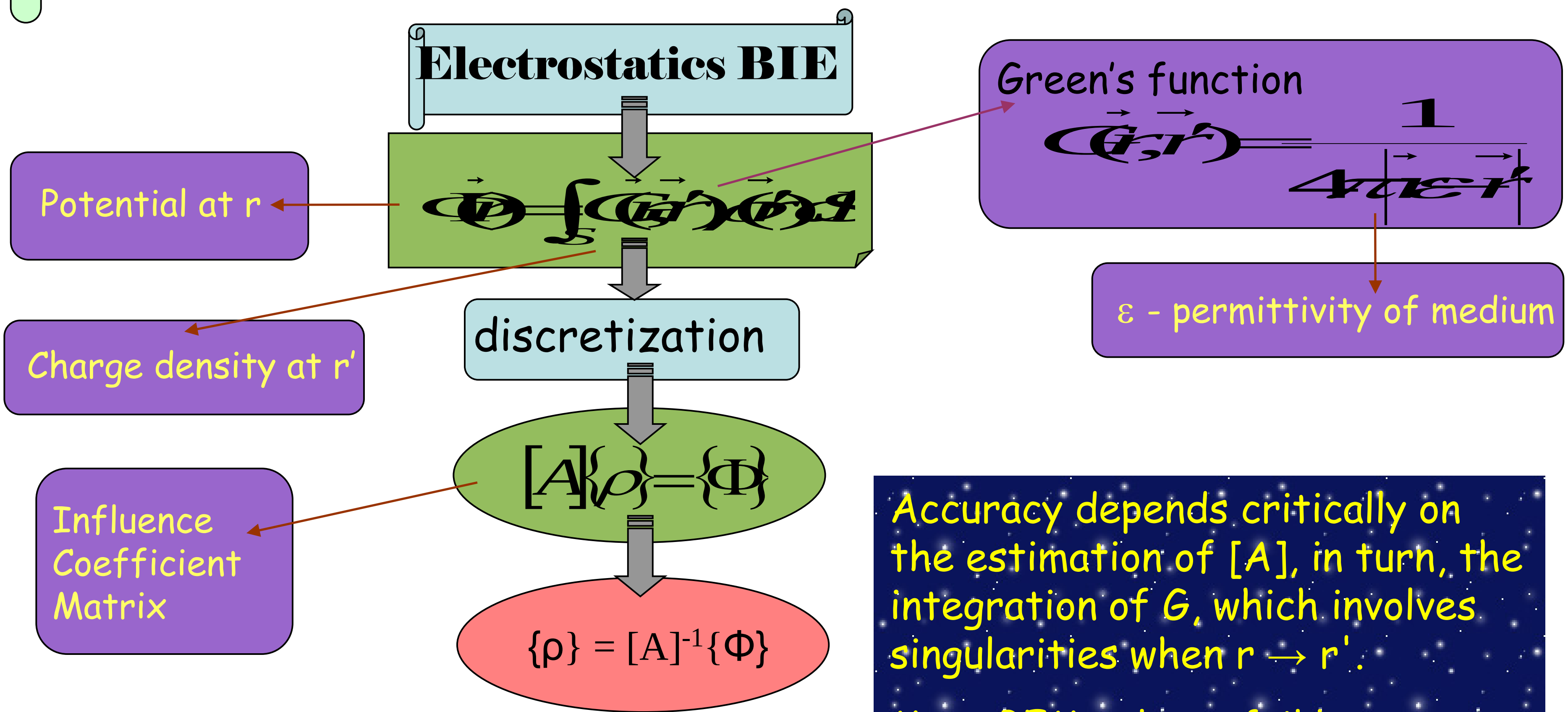
$$U_{2D} = (1/2\pi)\ln(r),\ U_{3D} = 1/(4\pi r),\ Q = -(1/2\pi\alpha r^{\alpha})\, r_{,n}$$

$\alpha = 1$ for 2D and 2 for 3D. Distance from *y* to *x* is *r*, n_i denoted the components of the outward normal vector of the boundary.

2D Case	3D Case	r = 0	$r \mapsto 0,\ r \neq 0$
ln(r)	1/r	Weak singularity	Nearly weak singularity
1/r	$1/r^2$	Strong singularity	Nearly strong singularity
$1/r^2$	$1/r^3$	Hyper singularity	Nearly hyper-singularity

BEM Solvers

- Numerical implementation of boundary integral equations (BIE) based on Green's function by discretization of boundary.
- Boundary elements endowed with distribution of sources, doublets, dipoles, vortices (singularities).
- Useful in fluid dynamics, fracture mechanics, acoustics, optics, gravitation, electromagnetics, quantum mechanics …



Accuracy depends critically on the estimation of [A], in turn, the integration of G, which involves singularities when r → r'.

Most BEM solvers fail here.

Conventional BEM

Major Approximations

- Singularities modeled by a sum of known basis functions with constant unknown coefficients.
- The strengths of the singularities solved depending upon the boundary conditions, modeled by shape functions.

Constant element approach

Singularities assumed to be concentrated at centroids of the elements, except for special cases such as self influence.

Boundary conditions are satisfied at the same nodal points.

Numerical boundary layer

Difficulties in modeling physical singularities

- geometric singularity
- boundary condition singularity

Conventional BEM

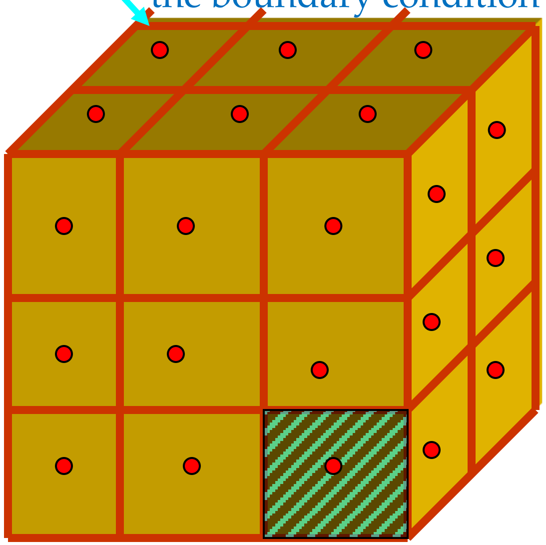
Basis Function Approach

Centroid Collocation

$$\Psi\left(x_{c_i}\right) = \sum_{j=1}^{n} \alpha_j \underbrace{\int_{panel\ j} \frac{1}{\left\| x_{c_i} - x' \right\|} dS'}_{A_{i,j}}$$

x_{c_i} Collocation point

Node where singularity is located and the boundary condition is satisfied



Single point quadrature

$$A_{i,j} \approx \frac{Panel\ \ Area}{\left\| x_{c_i} - x_{centroid_j} \right\|}$$

$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \vdots \\ \alpha_n \end{bmatrix} = \begin{bmatrix} \Psi\left(x_{c_1}\right) \\ \vdots \\ \vdots \\ \Psi\left(x_{c_n}\right) \end{bmatrix}$$

- Deals with nodal singularities and, thus, is plagued with the difficulties mentioned earlier
- Special treatment for self-influence.
- Number of special formulation to deal with critical problems such as such as with large length scale variations, closely packed surfaces, corners, edges and so on

nearly exact BEM

Using symbolic integration techniques, analytic expressions of potential and force field due to uniform distribution of singularities on flat *rectangular* and *triangular* elements have been obtained

Instead of nodal concentration of singularities, we now have,

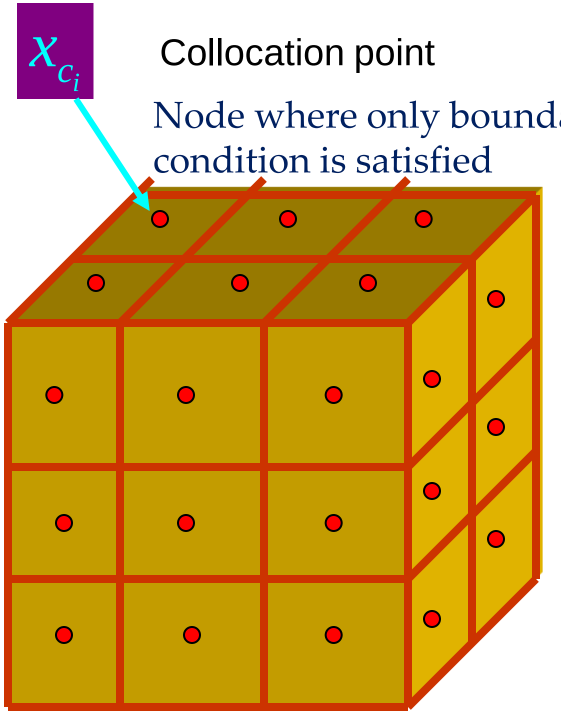
- Singularities distributed uniformly on the surface of boundary elements,
- Strength of the singularity changes from element to element,
- Strengths of the singularities solved depending upon the boundary conditions, modelled by the shape functions.

ISLES library and neBEM 3D Solver

Foundation expressions obtained through the integration of the Green's functions are analytic and valid for the complete physical domain

neBEM formalism

Basis Function Approach



Centroid Collocation

$$\Psi\left(x_{c_i}\right) = \sum_{j=1}^{n} \alpha_j \underbrace{\int_{panel\ j} \frac{1}{\left\| x_{c_i} - x' \right\|} dS'}_{A_{i,j}}$$

Carry out the integrations! $A_{i,j} = \int_S G(\vec{r}, \vec{r}') \rho(\vec{r}') dS'$

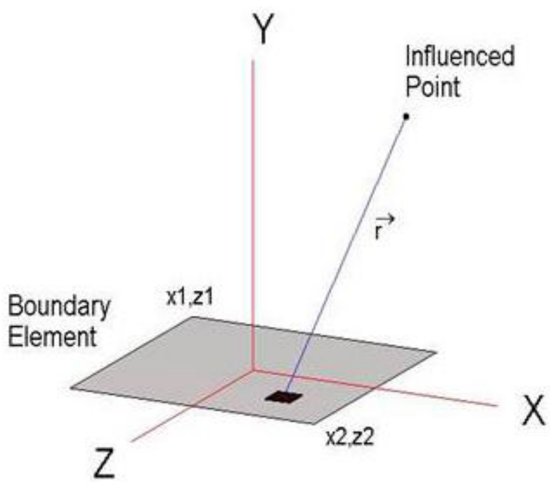
$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \vdots \\ \alpha_n \end{bmatrix} = \begin{bmatrix} \Psi\left(x_{c_1}\right) \\ \vdots \\ \vdots \\ \Psi\left(x_{c_n}\right) \end{bmatrix}$$

No singularities, no special treatments, no additional formulations! ☺

Foundation expressions of ISLES

Rectangular elements

Influence of a flat boundary element



$$\Phi(X,Y,Z)=\frac{1}{2}\times\left\{\begin{array}{l}2\times(X|Z|x_i|z_j)\times\ln\left(\frac{D_{i,j}-(X|Z-x_i|z_j)}{D_{m,n}-(X|Z-x_m|z_n)}\right)\\ +iS_j|Y|\times\left[\tanh^{-1}\left(\frac{R_j-iI_i}{D_{i,j}|Z-z_j|}\right)-\tanh^{-1}\left(\frac{R_j+iI_i}{D_{i,j}|Z-z_j|}\right)\right]\end{array}\right\}-2\pi$$

4 log terms

4+4 complex $\tanh^{-1}$ terms

$$D_{i,j}=\sqrt{(X-x_i)^2+Y^2+(Z-z_j)^2}$$

$$R_i=Y^2+(Z-z_i)^2$$

$$I_i=(X-x_i)|Y|$$

$$S_i=Sign(Z-z_i)$$

$$\Phi(X,Y,Z)=\int_{x1}^{x2}\int\frac{dx\,dz}{(X-x)^2+(Y-y)^2+(Z-z)^2}$$

Value of multiple dependent on strength of source and other physical consideration

May need translation and vector rotation

ISLES: Inverse Square Law Exact Solutions

Foundation expressions of ISLES

$$F_X(X,Y,Z)=\ln\left(\frac{D_{i,j}-(Z-z_j)}{D_{m,n}-(Z-z_n)}\right)$$

2 terms

$$F_Y(X,Y,Z)=$$

$$-\frac{i}{2}Sign(Y)\times\left\{\begin{array}{l} S_j\tanh^{-1}\left(\dfrac{R_j+iI_i}{D_{i,j}\left|Z-z_j\right|}\right)\\ +S_j\tanh^{-1}\left(\dfrac{R_j-iI_i}{D_{i,j}\left|Z-z_j\right|}\right)\end{array}\right\}+C$$

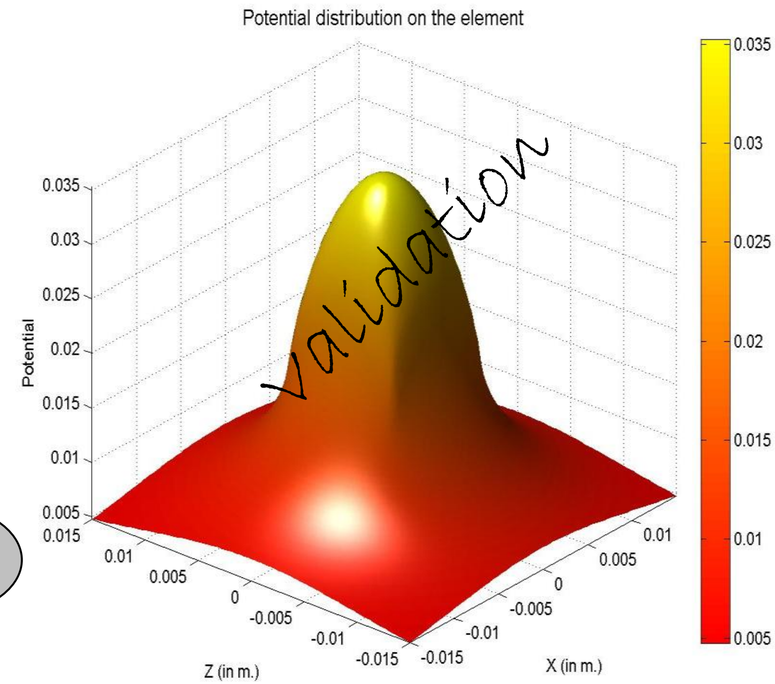
4+4 terms

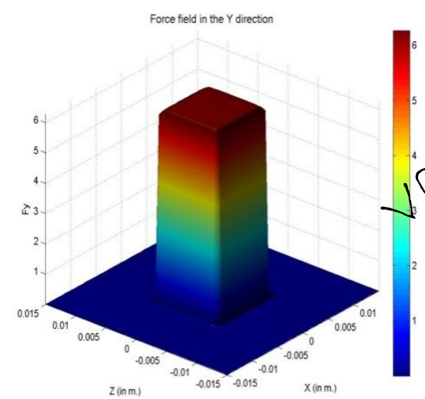
$$F_Z(X,Y,Z)=\ln\left(\frac{D_{i,j}-(X-x_i)}{D_{m,n}-(X-x_m)}\right)$$

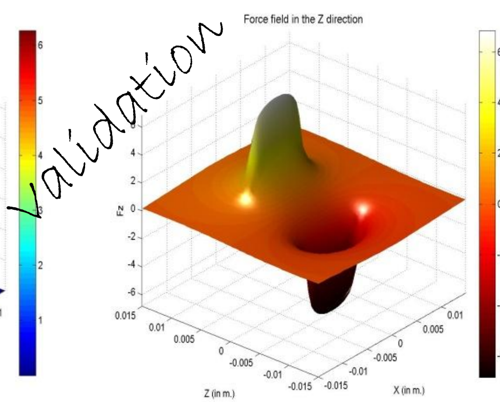
2 terms

C is a constant of integration as follows:

$$C=\begin{cases}0, & \text{if outside the XZ extent of the element}\\ 2\pi, & \text{if within, and } Y>0\\ -2\pi, & \text{if within and } Y<0\end{cases}$$



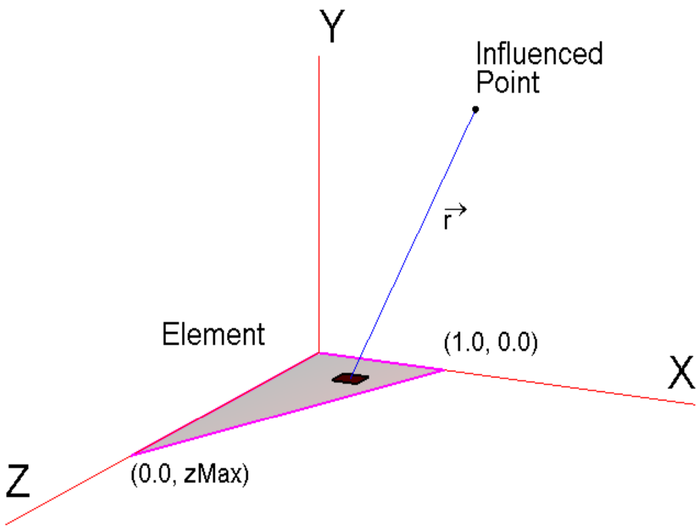




Foundation expressions of ISLES

Triangular elements

Influence of a flat triangular element



$$\Phi(X,Y,Z)=\int_0^1\int_0^{z(x)}\frac{dxdz}{\sqrt{(X-x)^2+(Y-y)^2+(Z-z)^2}}$$

Similar expressions as for rectangular elements but much longer

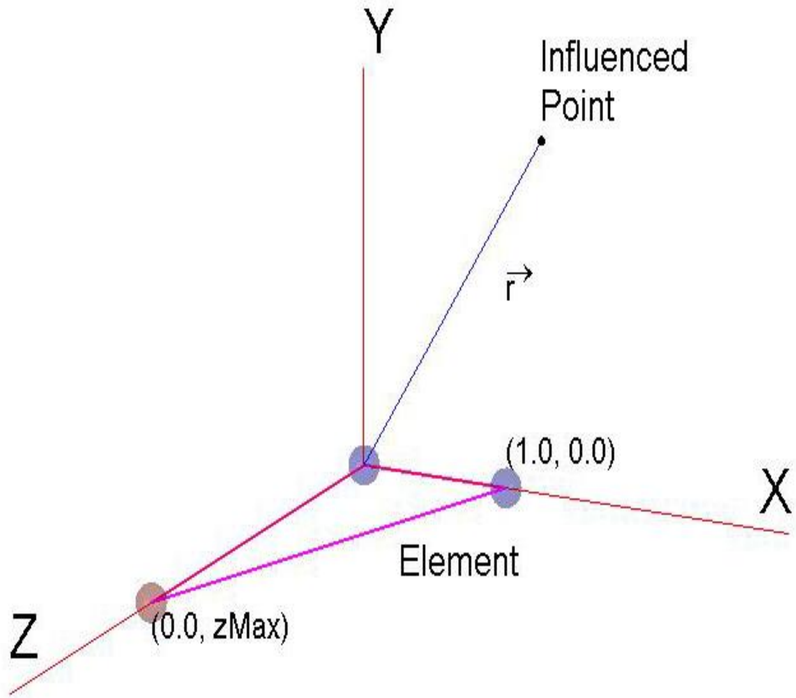
- Two parameters are important: precision and speed
- For the evaluation of accuracy, we have computed the influence at a given point by further discretizing the triangular element into small rectangular elements
- Evaluation of speed has been carried out using the Linux / UNIX system routine "gprof"
- From the study we have concluded that the accuracy achieved more than justifies the extra computation

May need translation, vector rotation and simple scalar scaling

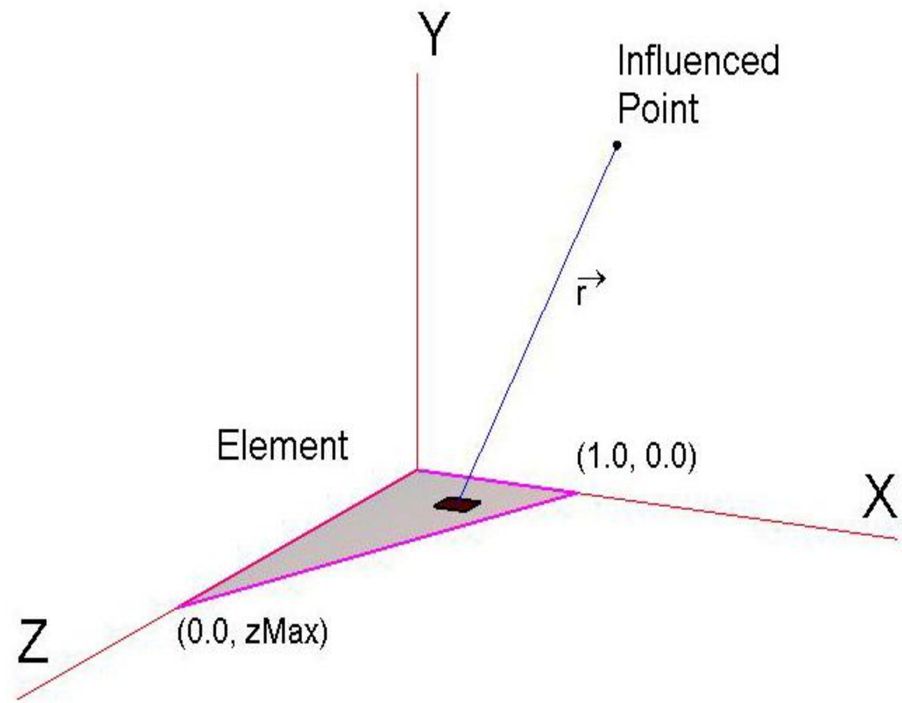
Contrast of approaches

nodal versus distributed

Influence of a flat triangular element in Usual BEM



Influence of a flat triangular element in ISLES



Contrast of approaches

Influence of a flat triangular element in Usual BEM

- ✓ Easily implemented
- ✖ Numerical boundary layer
- ✖ Inaccurate near field
- ✖ Closely spaced elements intractable
- ✖ Computationally expensive

Influence of a flat triangular element in ISLES

- ✓ Accurate in the near field
- ✓ Computationally efficient
- ✖ Previous approaches were extremely difficult to implement
    - Hess and Smith (67) needs in-plane projections and evaluation of complicated expressions
    - Newman (84) needs application of Gauss-Bonnet theorem and evaluation of complicated expressions
- ✓ ISLES is as accurate and straight-forward to implement

Intermediate approaches such as Dual reciprocity BEM, Extended BEM, Thin plate BEM:

- ✓ Accurate within the range of validity
- ✖ Valid for a specific set of problems
- ✖ Complicated mathematics

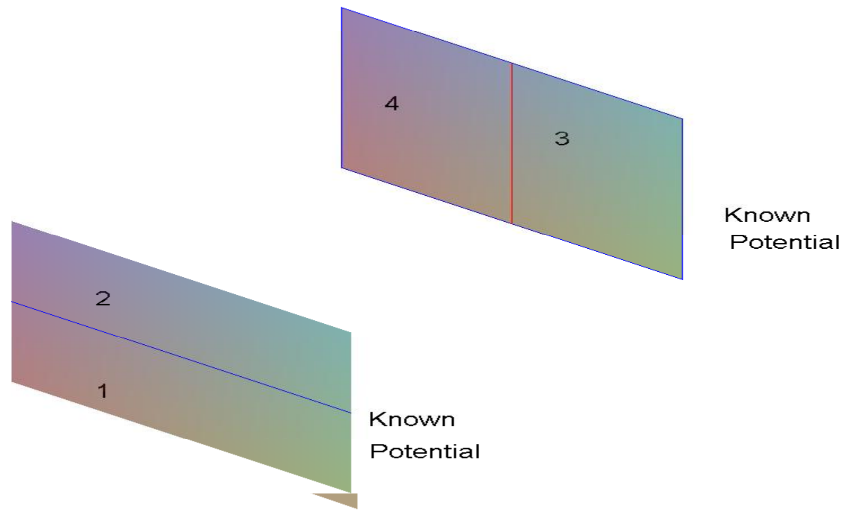
Floating conductors – an example of a constrained solution

- Several approaches, following one of the more efficient, used commonly for `dummy fills' in integrated circuits.
- Two properties of the floating conductors are exploited
  - A uniform potential will be created on each floating conducting particle due to the charges induced on it. This potential may vary from one floating particle to another.
  - For a given floating conducting particle, the sum of all charges induced on the particle is zero.
- This translates as additional one column and one row for each floating conductor in the system to modify the system of algebraic equations representing the physical situation.
- Rest is usual.
- It is similarly possible to constrain a solution in order to satisfy other Physics requirements.

Floating conductors

A simple example

Problem with one floating conductor



- Consider a system of two conductors, each having been discretized into two elements.
- One of these conductors is at a known voltage, V. The other conductor is at a floating voltage V_F, which is unknown.
- Number the elements on the conductor with known voltage to be 1, 2, and those on the floating conductor to be 3, 4.
- Denote charge densities by ρ_i, area by A_i, on each element
- Resulting system of equation is as shown.
- In the above system, I_{ij} denotes the influence of the jth element on the ith element.
- Please note that if we have more than one floating conductor, they cannot be assumed to be at the same potential, and one column and one row as shown above needs to be added for each floating conductor.

$$\begin{bmatrix} I_{11} & I_{12} & I_{13} & I_{14} & 0 \\ I_{21} & I_{22} & I_{23} & I_{24} & 0 \\ I_{31} & I_{32} & I_{33} & I_{34} & -1 \\ I_{41} & I_{42} & I_{43} & I_{44} & -1 \\ 0 & 0 & A_3 & A_4 & 0 \end{bmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \\ \rho_4 \\ V_F \end{pmatrix} \equiv \begin{pmatrix} V \\ V \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Objects with known charge density

- Easy to take these into account
- Only the right-hand side changes, the influence matrix remaining unchanged
- It is convenient to use big, and as a result, less number of elements because of the new foundation expressions
- The resulting computation is very efficient
- At present, it is possible to consider the effects of point, line and surface charges in the nearly exact sense. Work on an improved model for volume charges (space charges) is on at a very high priority (more on this later)

Recent developments

Complete and almost done!

Topics

- Repeated structures
- Weighting field
- New / reuse model
- Discretization controls
- Wire primitives
- Mirror reflections

Repeated structures

- It is difficult to evaluate the influence matrix for periodic structures.
- A simpler approach was adopted in which primitives are allowed to be repeated appropriate number of times in X, Y or Z directions.
- The direction can be arbitrary, but at present repetition only in these three directions has been implemented.
- The major approximation that the user has to be aware is, while using repetition, it is not only the geometry that is being copied, but also the charge density. This is natural for periodic structures.
- The computational advantage is huge. While the computation of influence coefficient matrix is longer, the influence matrix is much smaller and the resulting matrix inversion time is smaller by orders of magnitude!
- Interface has been completed and functional.

Weighting Field

- Efficient computation of weighting field has been implemented.
- The influence matrix is inverted only once and kept in memory or in the form of a stored file.
- Depending on the selected electrode(s), necessary rows of the inverted matrix is simply added to provide the charge density associated when the selected electrodes are raised to 1.
- From the obtained solution (charge density), weighting field at any point can be easily obtained.
- Interface has been completed.

New / Reuse Model

- Storage of influence coefficient matrix, inverted matrix
- Storage of primitives and elements have been added
- It should be possible to Reuse earlier solutions
- Can be very useful for trying out new voltage configurations for the same device geometry
- Interface working, although there can be small modifications in the immediate future.
- Formatted files are being used at present. We need to shift to unformatted files, as soon as possible.

Discretization controls

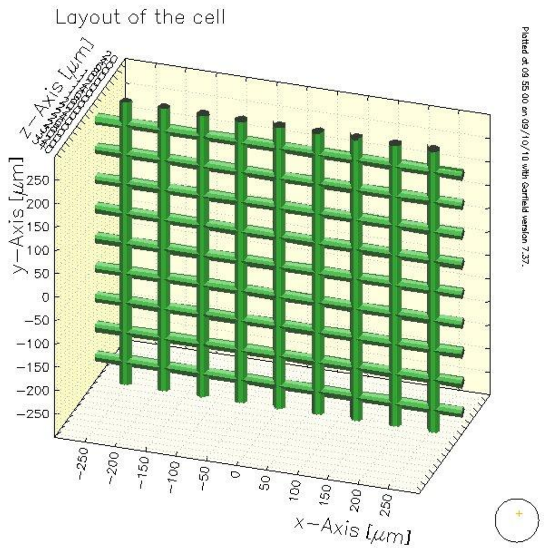
- Some modifications have been made in the way a user controls the discretization
- Target element size can be specified
- Maximum and minimum number of elements on each primitive can be specified
- Number of elements on a primitive (varying from primitive to primitive) can be specified
- Needs significant improvement – has to be made adaptive
- Interface present and woring.

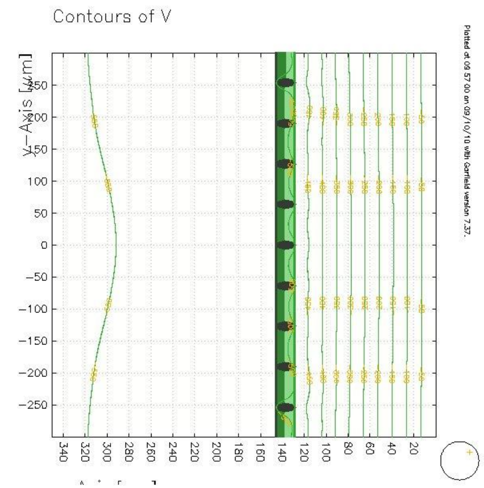
Wire Primitives

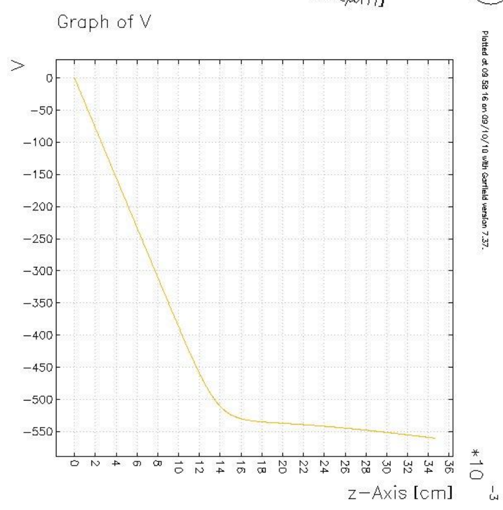
- Wires of finite length can be added as components of a device
- They can be of any orientation
- Wires can be modeled as thick wire (cylinders)
- If length >> radius, they can be modeled as thin wires
- Thin wires are very efficient computationally
- Small issues related to repetition of wire primitives has been sorted out
- Interface present and working

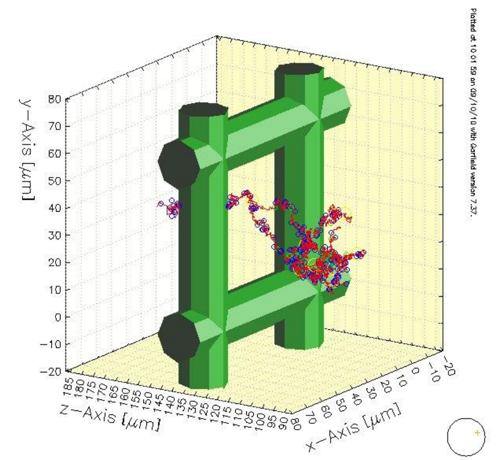
Wire mesh without repetition

- The script is long
- The voltage contour near drift plane should be flat
- No other problem observed at the moment



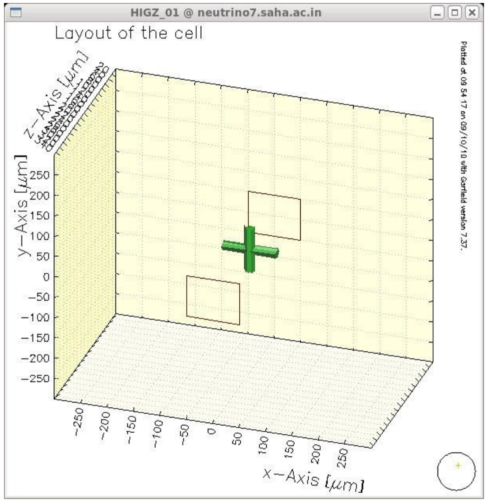


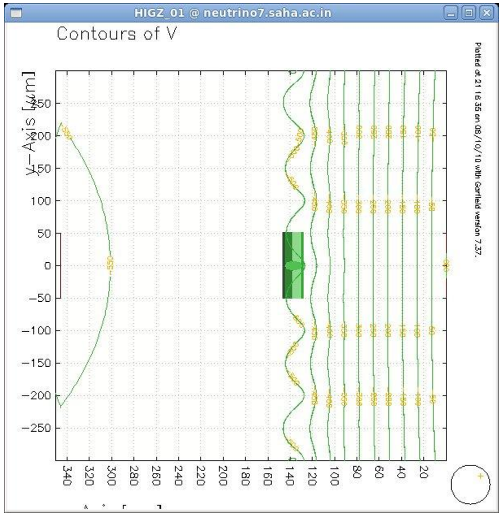


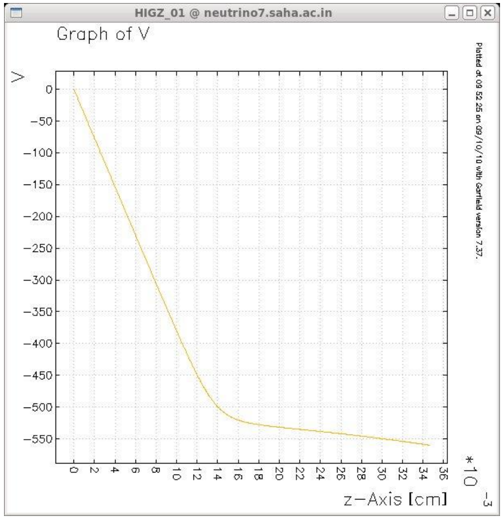


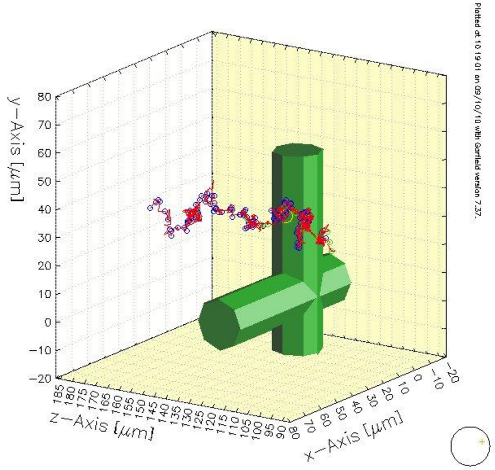
Wire mesh with 5 repetitions

- The script is long
- The voltage contour near drift plane should be flat
- No other problem observed at the moment



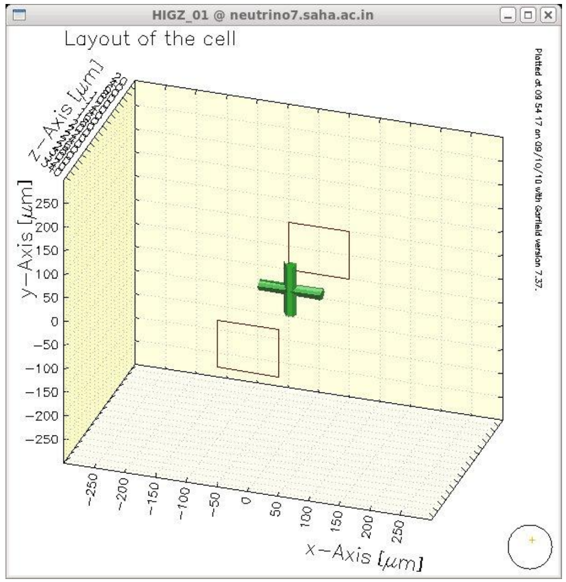


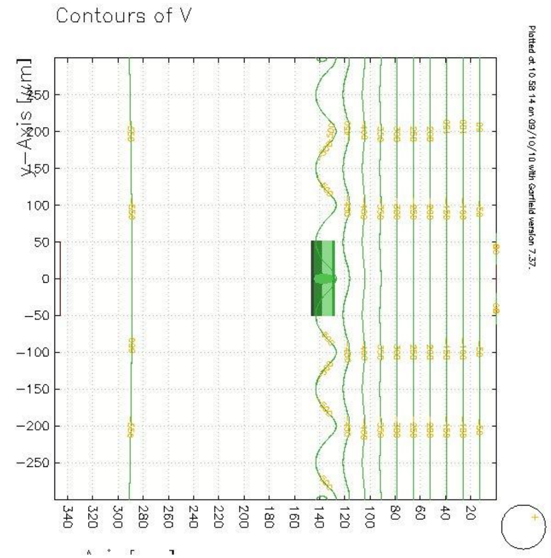


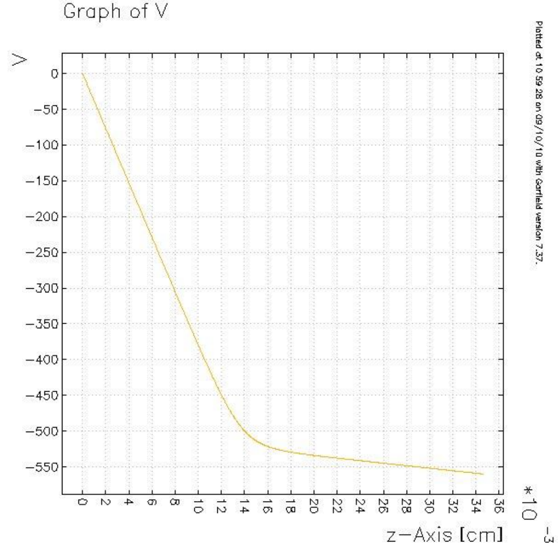


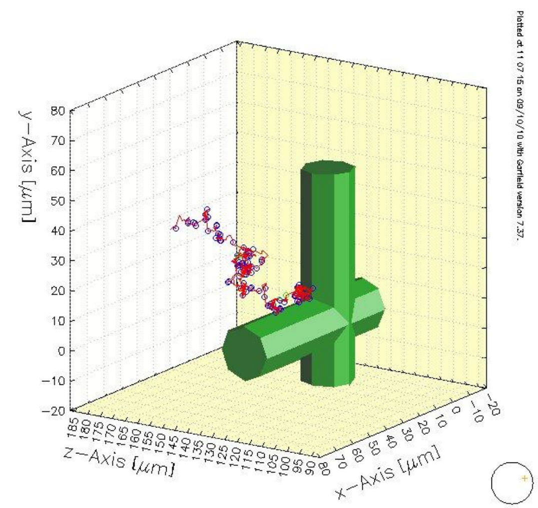
Wire mesh using 20 repetitions

- The script is short
- The voltage contour near drift plane very flat
- Takes longer time
- No other problem observed at the moment









Mirror Reflection

- Added very recently
- Mirrors normal to X, Y and Z are allowed
- Some very basic tests have been found to be satisfactory
- Integration to the interface yet to be completed
- Work on mirrors at arbitrary orientation can be pursued, if necessary
- Capacitance of a square flat plate at 1 V: 0.3667
- Rough Calculation:

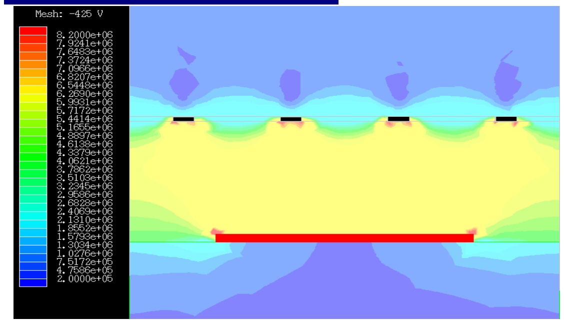
Full Plate	0.363708
Half Plate(X Mirror)	0.181854
Half Plate (Y Mirror)	0.181854
Half Plate (Z Mirror)	0.181854

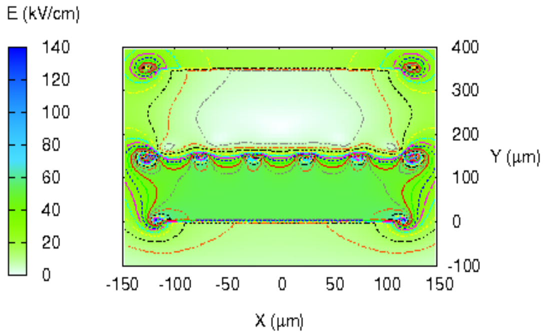
Applications

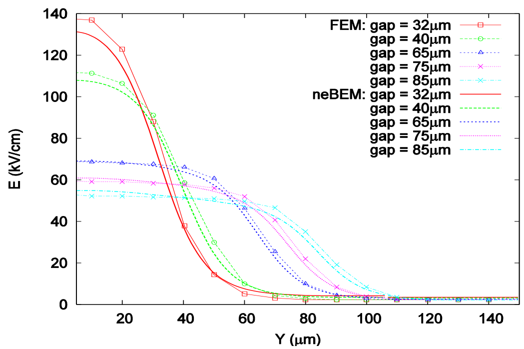
MPGDs and Others

Electrostatics of MPGDs

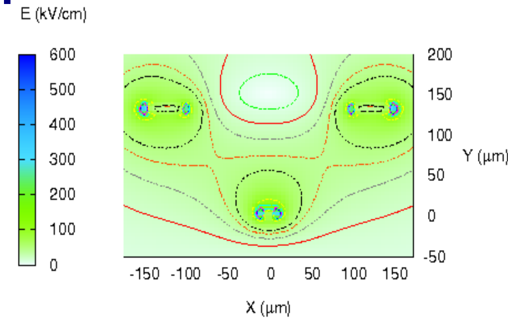
Micromegas

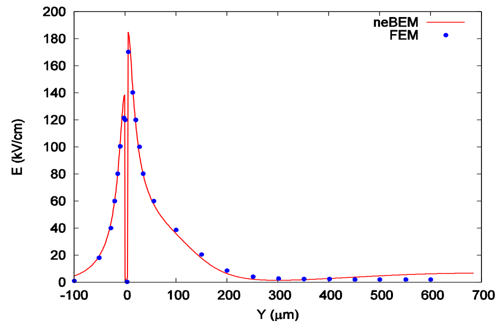


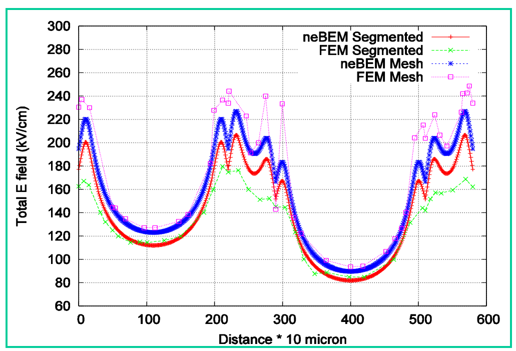




Micro-Wire





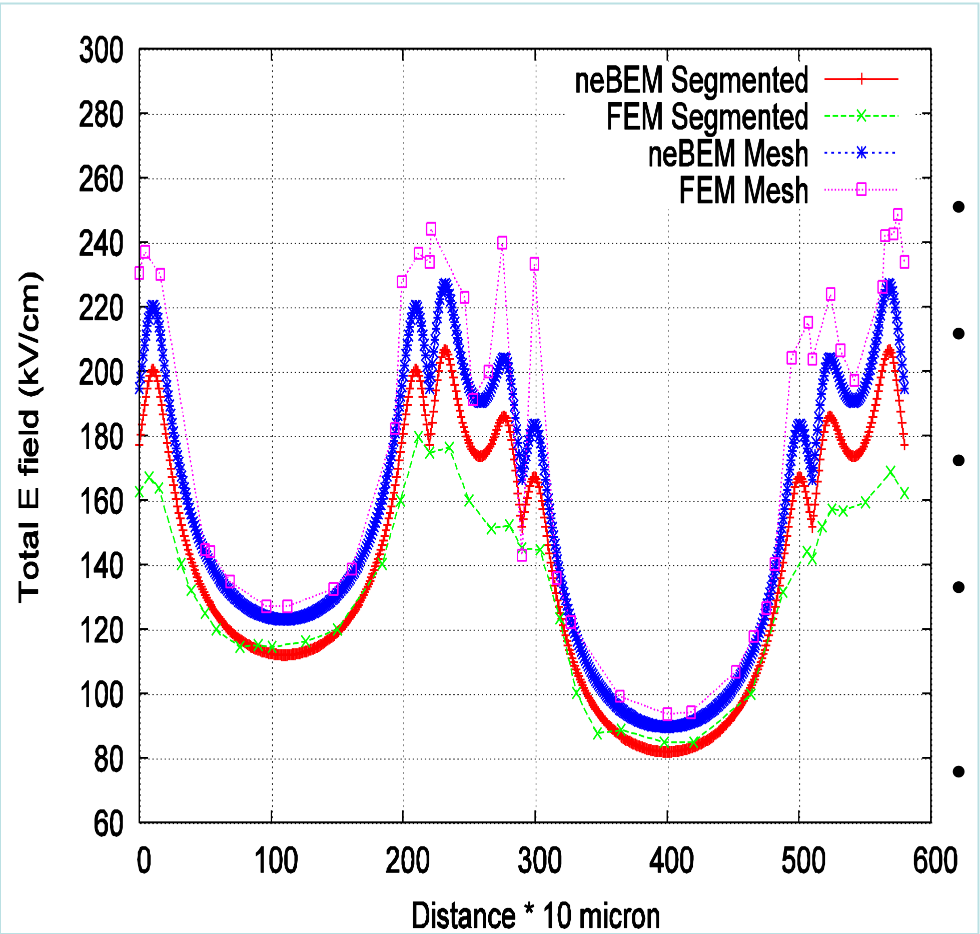


Theoretical considerations imply better performance by the neBEM solver which solves for the charge density on boundary elements rather than potential at a pre-fixed set of nodal points.

Numerical comparisons
1) neBEM results are as accurate as FEM results in the far-field
2) In the near-field, neBEM performs better than FEM
3) No artificial truncation of open domain is necessary while using neBEM

Comparison with FEM

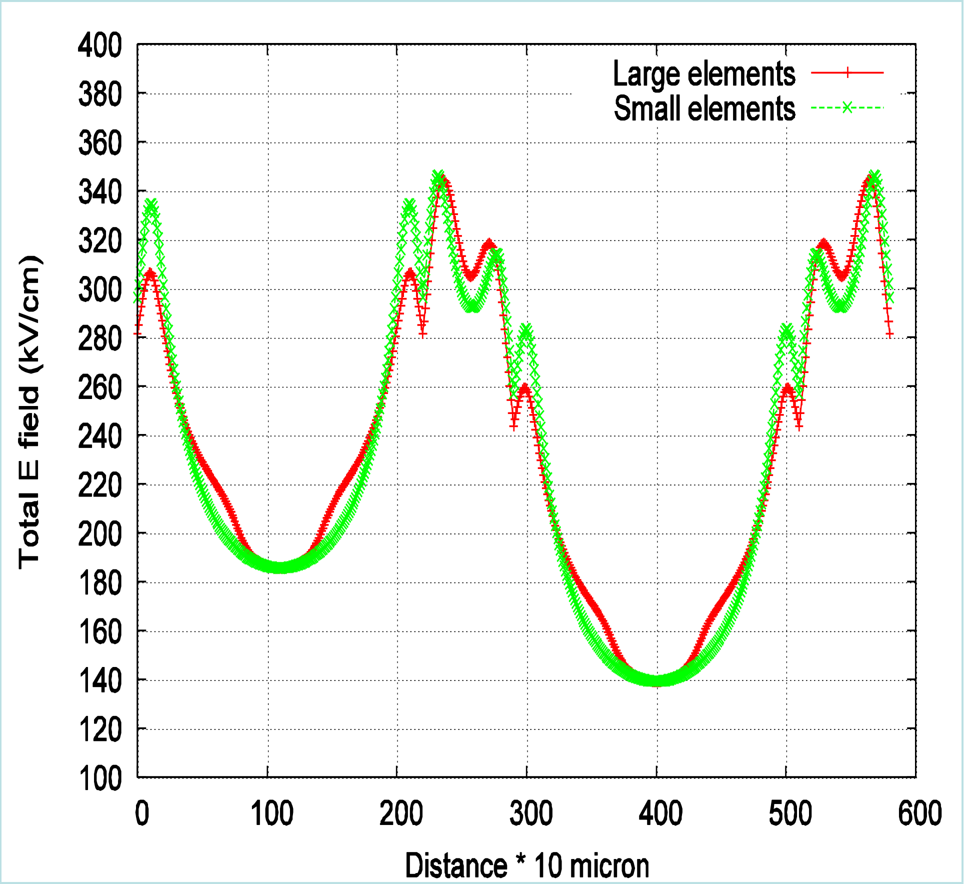
Near-field



- Field around a line just 1μm away from the anode surface is considered here – sampling for neBEM is as small as 0.1μm!
- The mesh configuration has higher field values throughout
- Sharp rise in the field values is observed at all the four edges
- Smooth variation of field is observed on each of the four surfaces
- Field values are found to decrease sharply once the points are beyond anode surfaces
- FEM computation is clearly unable to produce correct results near and at the edges
- FEM, although better on the surfaces, still falls behind neBEM in performance

Effect of discretization

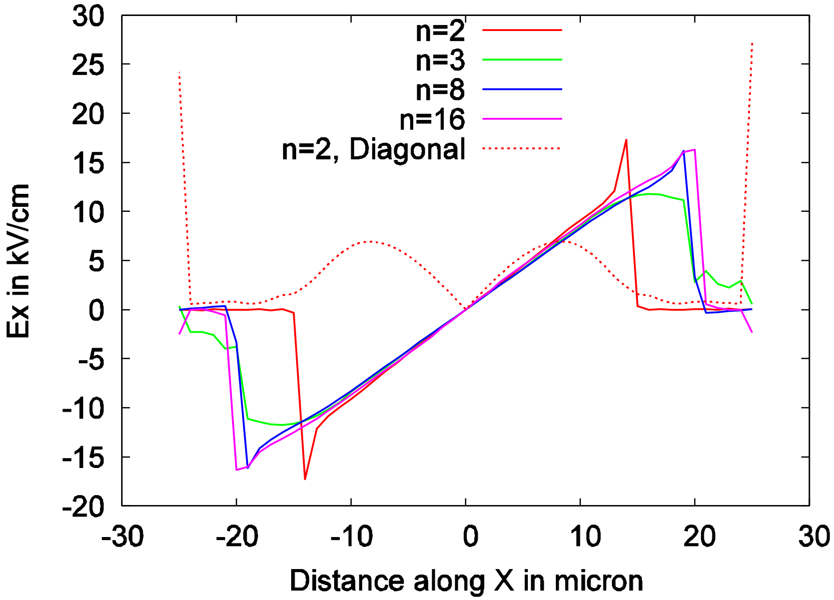
Near-field



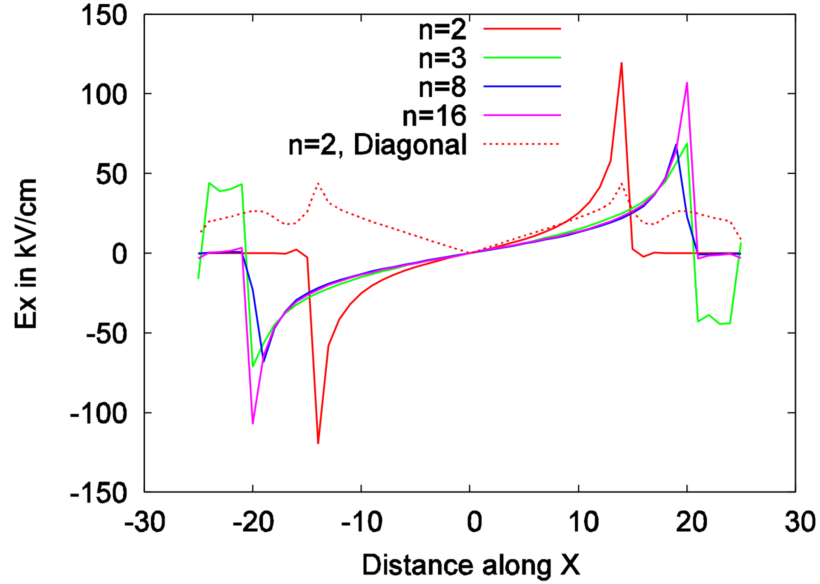
- In the earlier computation, we had used 20 elements to represent the top surface and 10 elements on the side surface. The elements were made successively smaller towards the edges
- In order to study effect of using coarse discretization, we also used larger elements of fixed size – only 3 elements each to represent both top and side surfaces
- Although there is significant difference between the results, the overall trend is represented well by the larger elements
- It is important to note that there is no jaggedness (at 0.1μm sampling) despite the use of unreasonably large elements!

Microscopic details in Micromegas

Variation of transverse electric field on the mesh surface along the transverse direction for four different shape of mesh hole



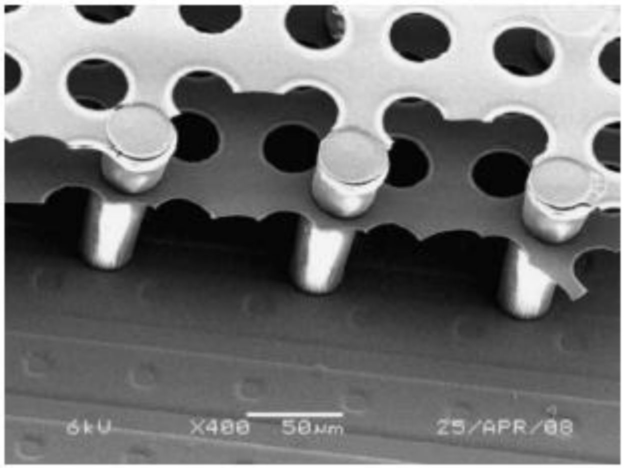
Surface side in the drift region

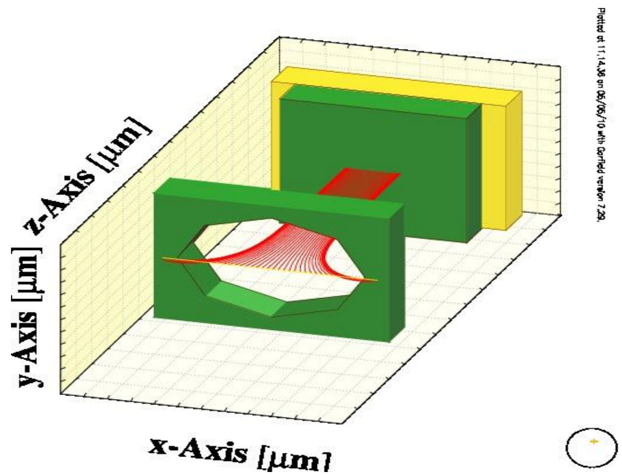


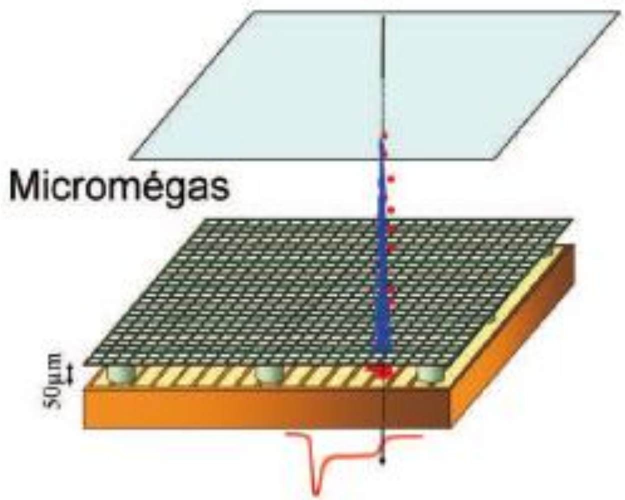
Surface side in the amplification region

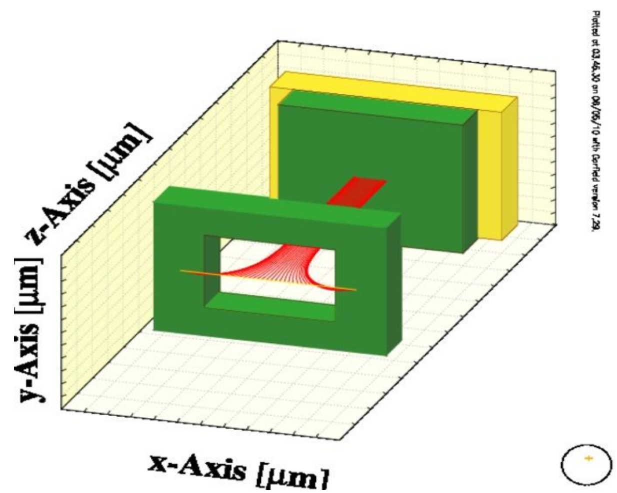
- The transverse electric field is significant close to the edge
- Possibility of discharges, again.

Garfield+neBEM+Magboltz+Heed
Micromegas







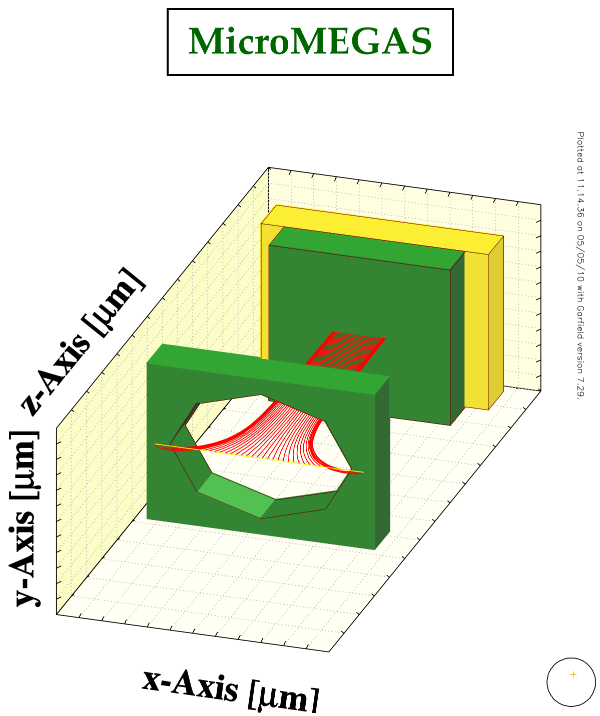


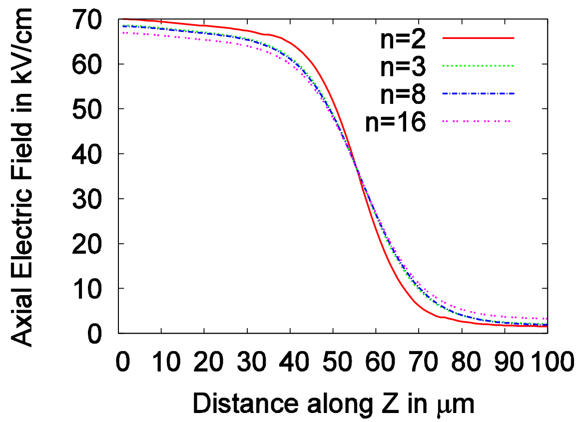
Role of different geometrical models for the same device

NIM A (2010) (in press) (doi: 10.1016/j.nima.2010.07.026)

"Realistic three dimensional simulation on the performance of micromegas"

P. Bhattacharya, S. Mukhopadhyay, N. Majumdar, S. Bhattacharya





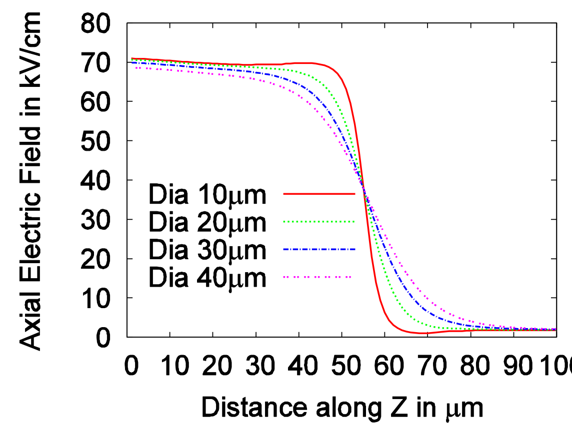


Table 2: Variation of gain with hole-shape

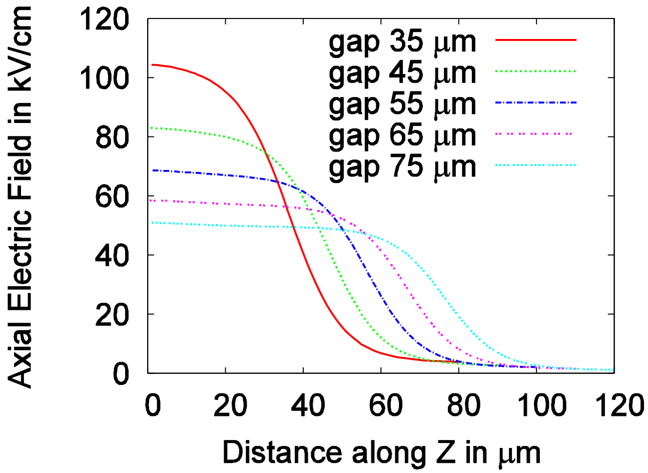
Hole-Shape	Gain, using Garfield
$n = 2$	1220
$n = 3$	980
$n = 8$	890
$n = 16$	770

Table 3: Variation of gain with hole-size

Hole diameter (μm)	Gain, using Garfield
10	1900
20	1600
30	1250
40	980

Gas composition: 90% Argon + 10% Isobutane
Temp.: 300 K, Pressure : 1 Atm

MicroMEGAS



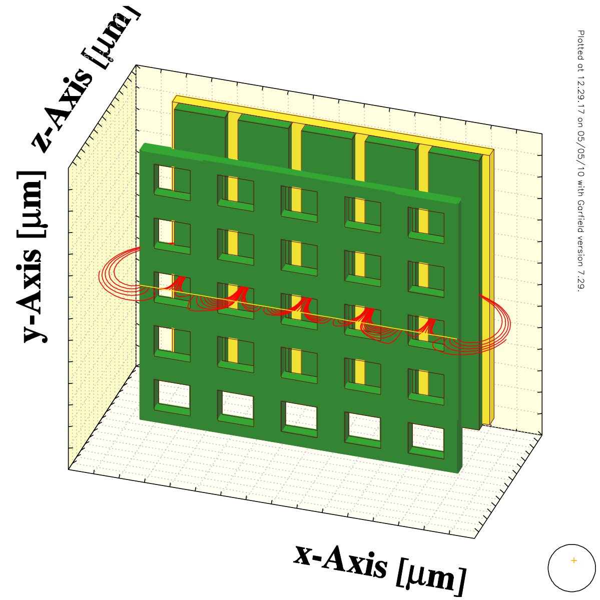
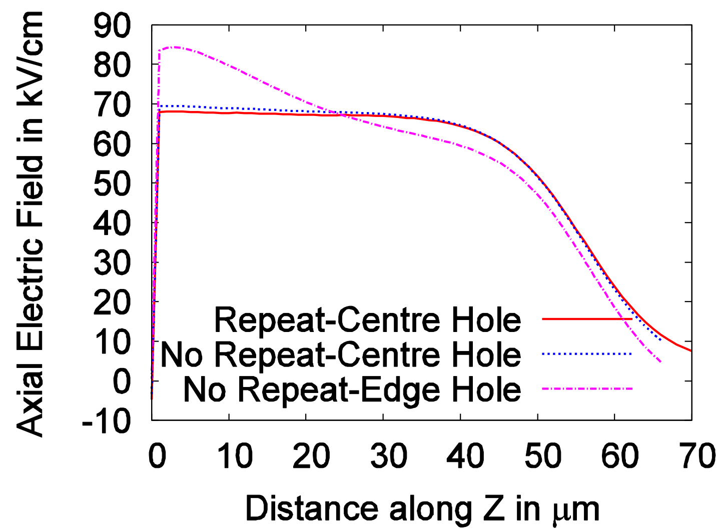


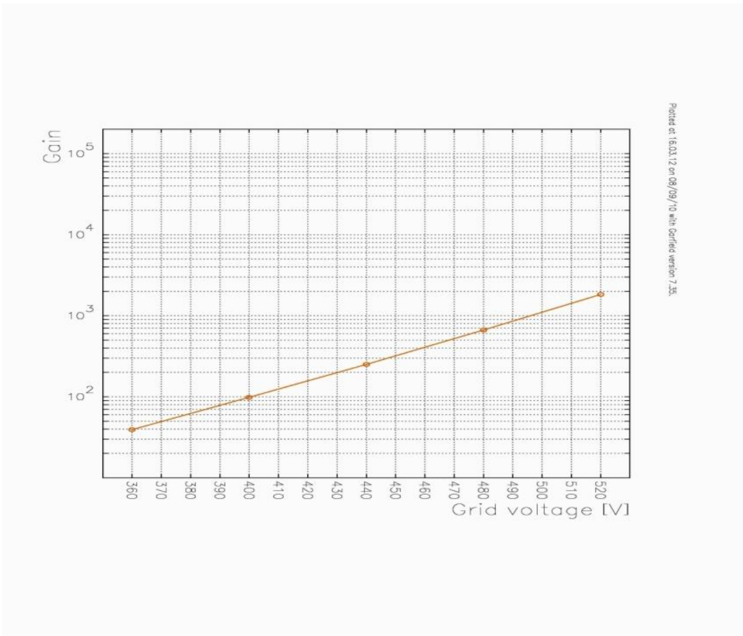
Table 5: Variation of the gain with amplification gap

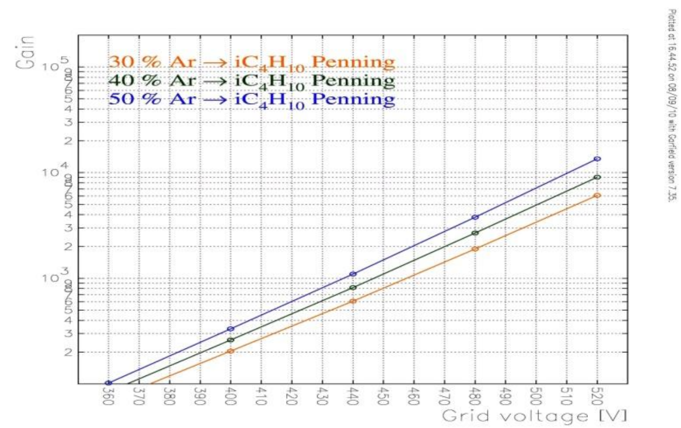
Amplification Gap (μm)	Gain, using Garfield
35	2500
45	1550
55	980
65	610
75	380

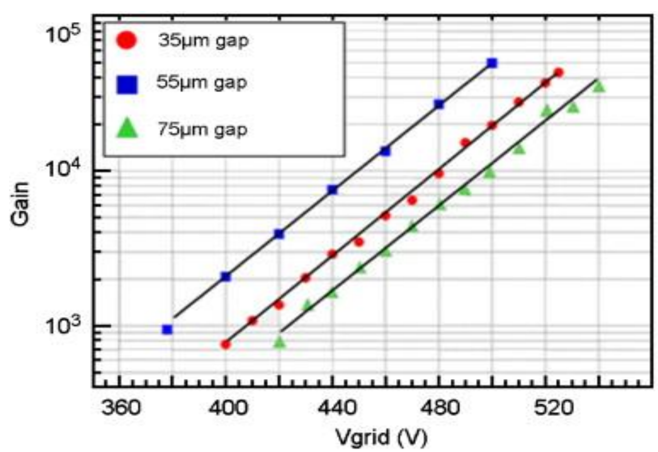


Garfield+neBEM+Magboltz+Heed

Micromegas



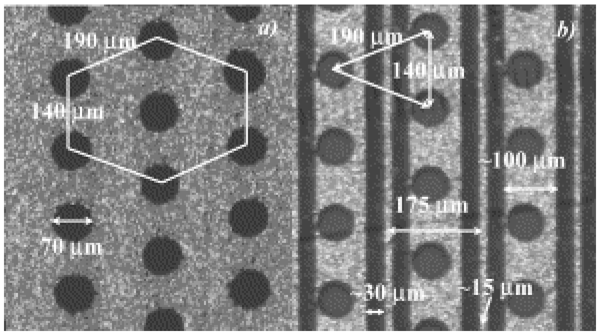


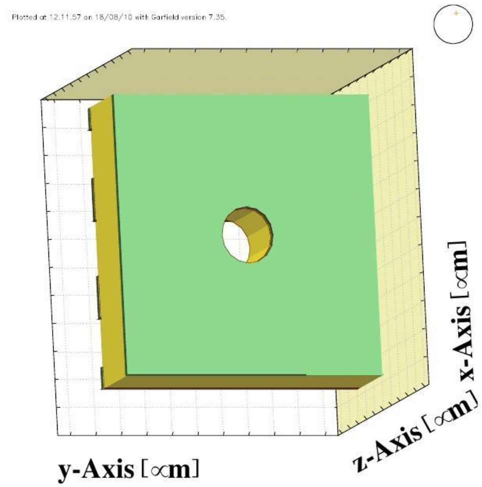


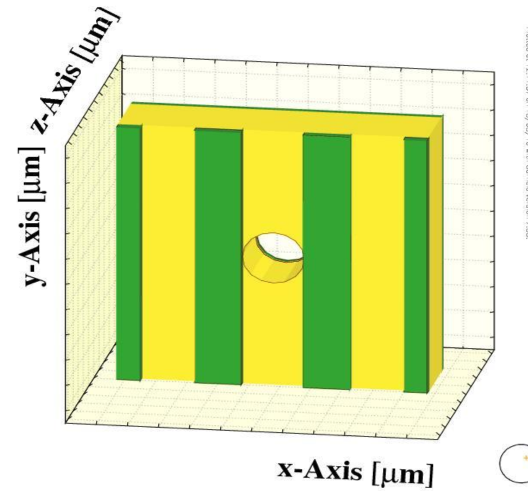
Roles different parameters are likely to play:
Here we toy with the percentage of Penning Transfer
Similar Physics processes could be Multiple Scattering, Delta Ray production and so on …

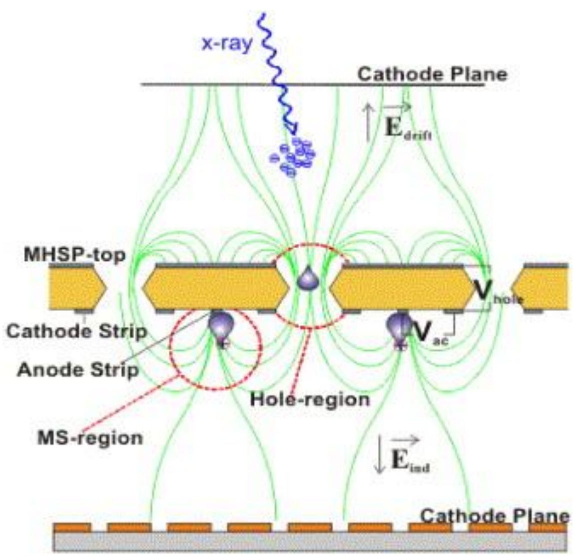
Garfield+neBEM+Magboltz+Heed

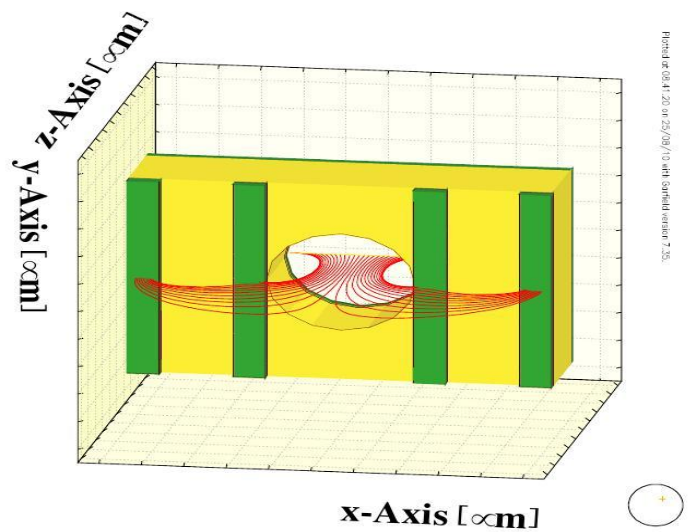
MicroHoleStripPlate





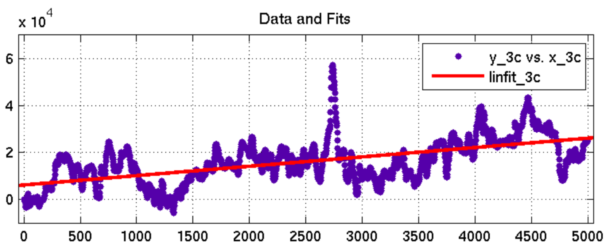


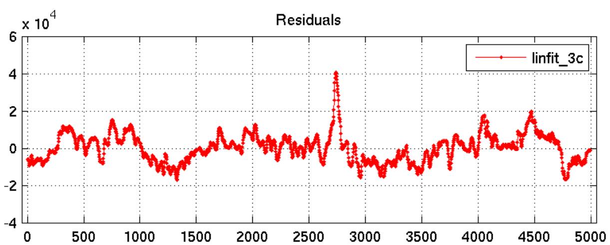




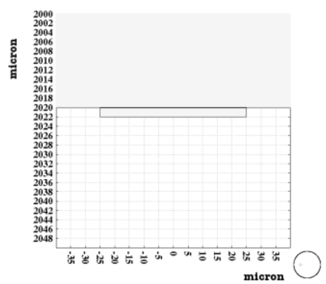
Surface asperities:

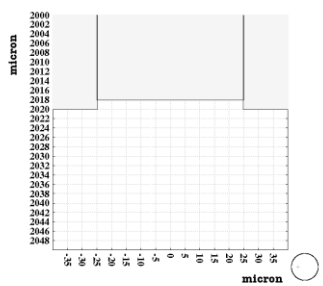
Influence of the surface asperities of the resistive electrode on the field configuration

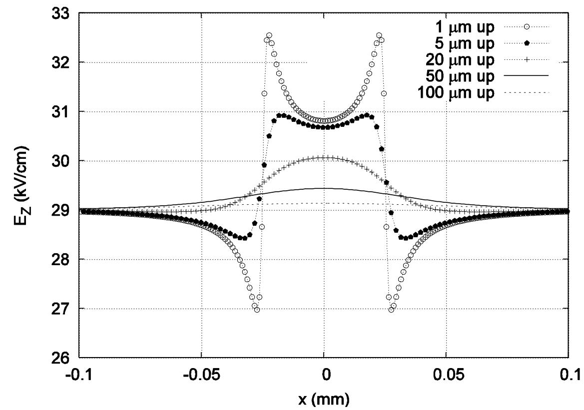




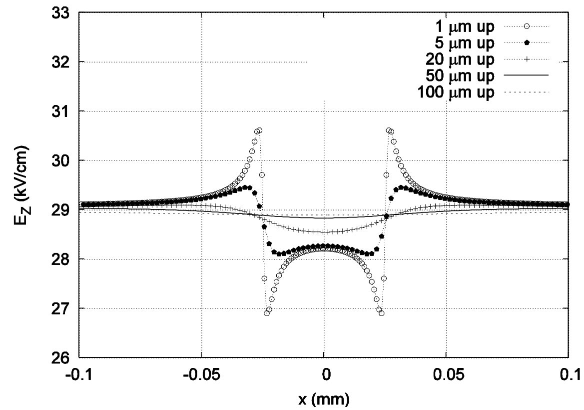
Modeled asperities







+ve asperity

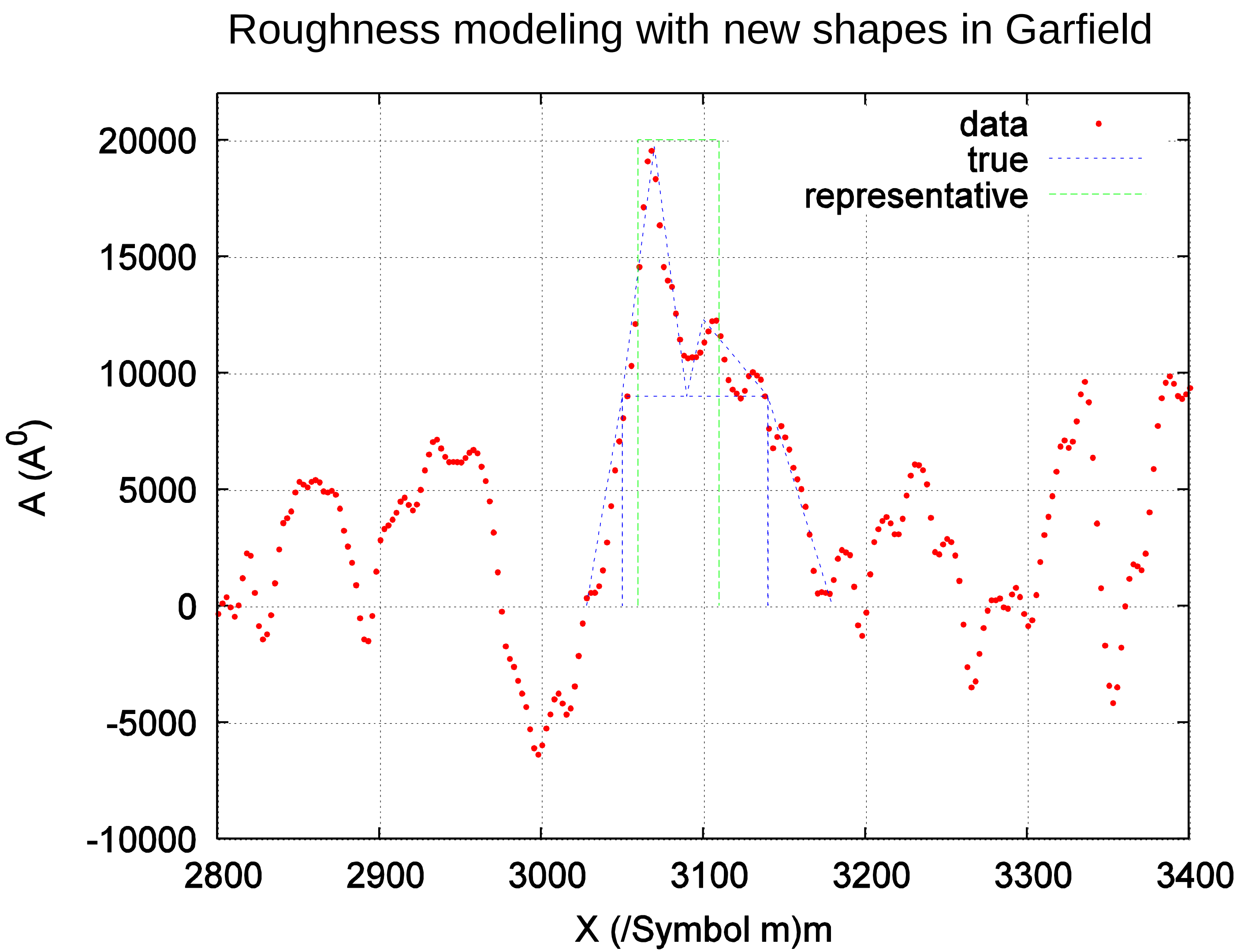


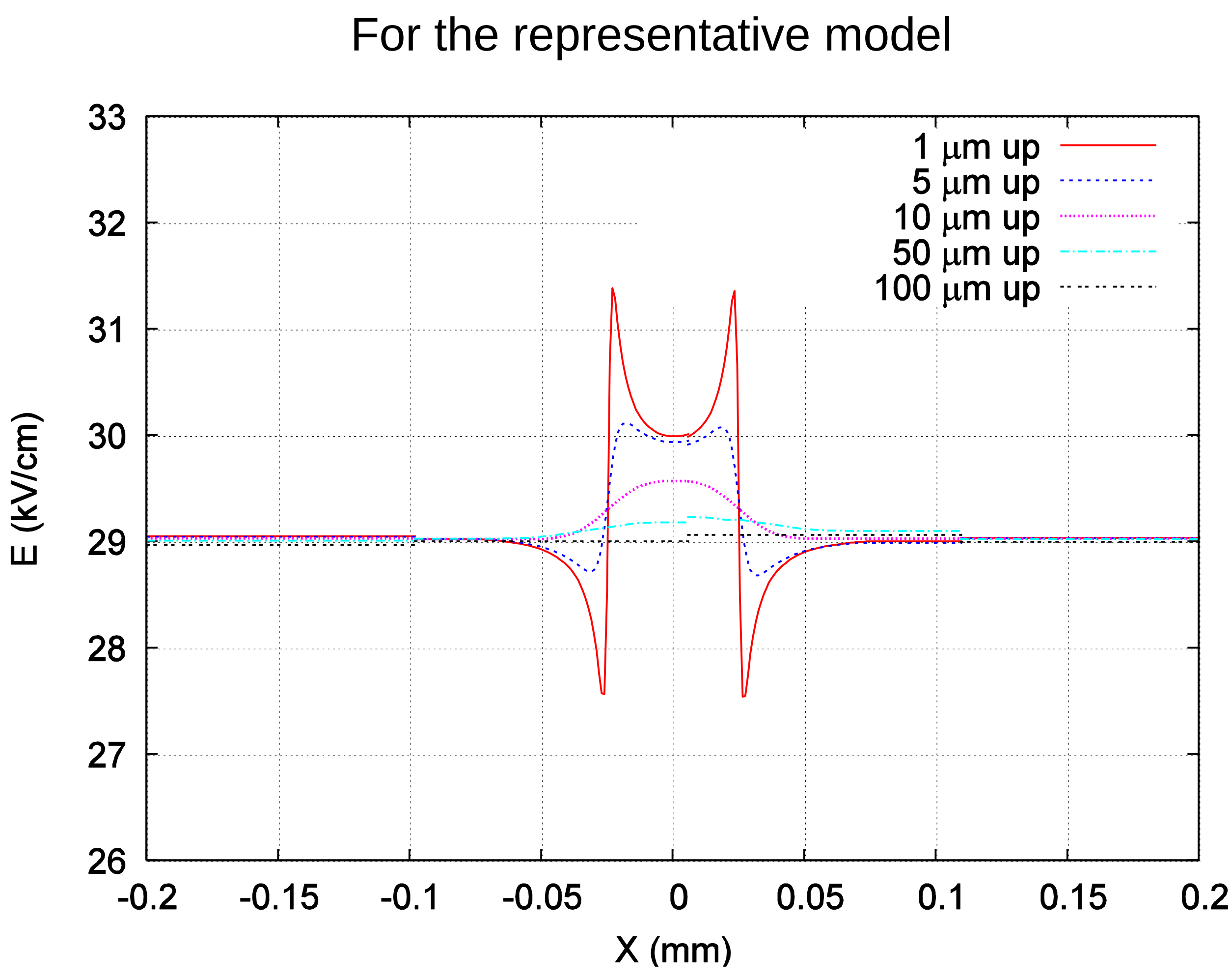
-ve asperity

NIM A (doi: 10.1016/j.nima.2010.09.168)

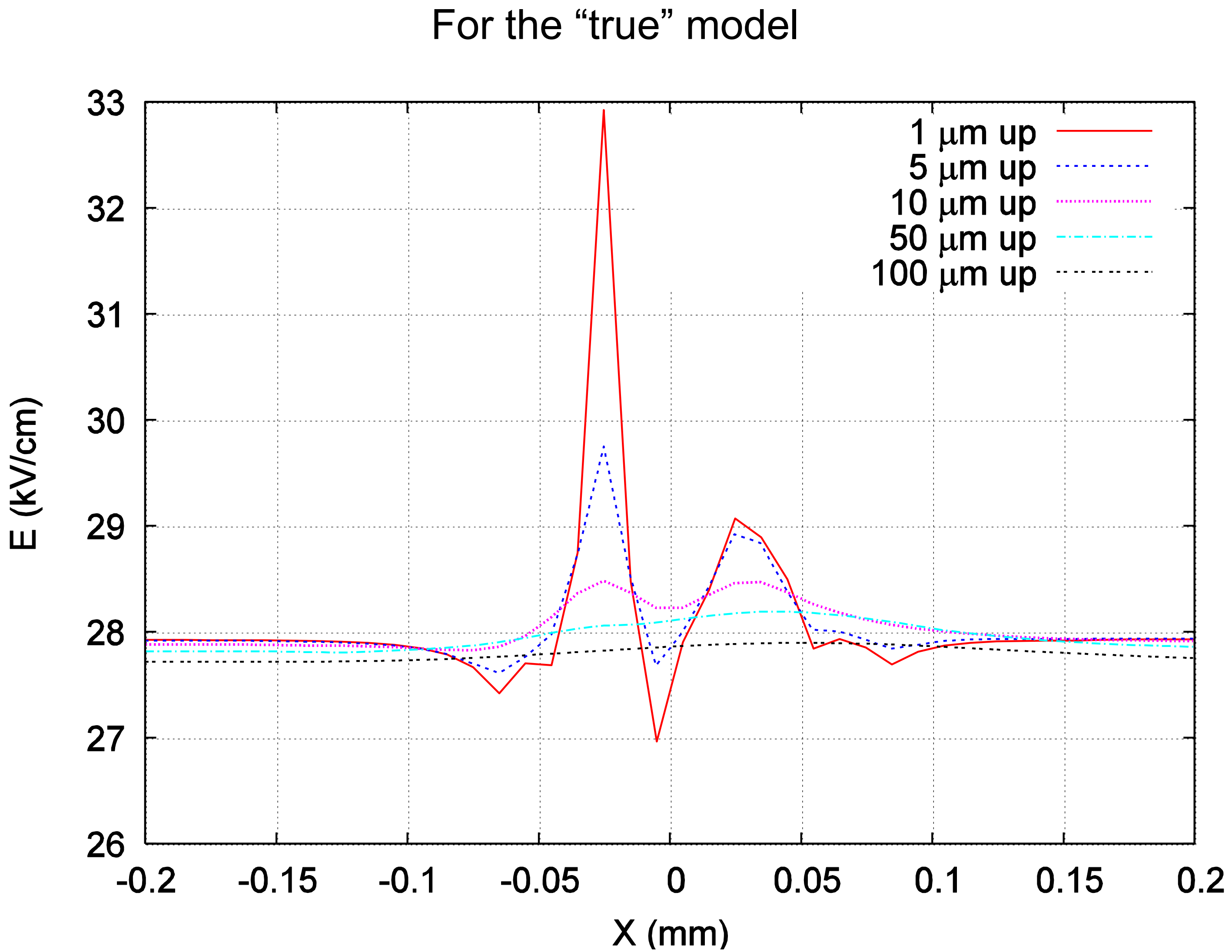
"Performances of silicone coated high resistive bakelite RPC"

S. Biswas et al.


Roughness modeling with new shapes in Garfield
data
true
representative
20000
15000
10000
5000
0
-5000
-10000
2800
2900
3000
3100
3200
3300
3400
A (A^0)
X (/Symbol m)m



For the representative model
1 μm up
5 μm up
10 μm up
50 μm up
100 μm up
33
32
31
30
29
28
27
26
E (kV/cm)
-0.2
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
0.2
X (mm)


For the "true" model
E (kV/cm)
X (mm)
1 μm up
5 μm up
10 μm up
50 μm up
100 μm up
33
32
31
30
29
28
27
26
-0.2
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
0.2

Ongoing developments

In lieu of a future plan

Topics

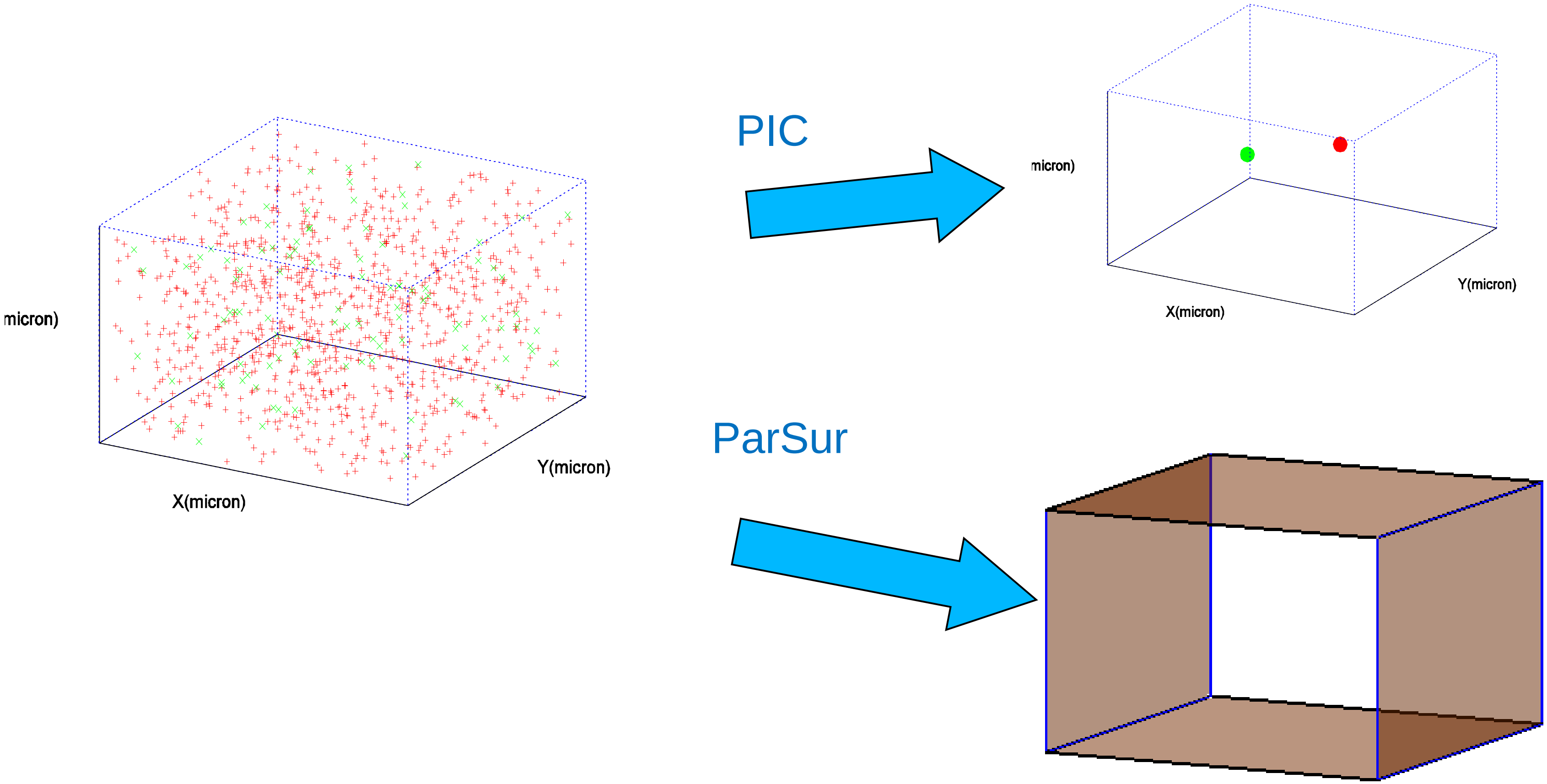
- Known charges
- Space charge
- Adaptive meshing
- Parallelization

Effect of known charge

- Known point, line and surface charges can be modeled efficiently.
- Only the RHS of the matrix system gets modified, as explained earlier
- Can be very useful for dynamic problems such as charging up
- Needs more work
- Interface to be developed

Particles on Surface (ParSur)

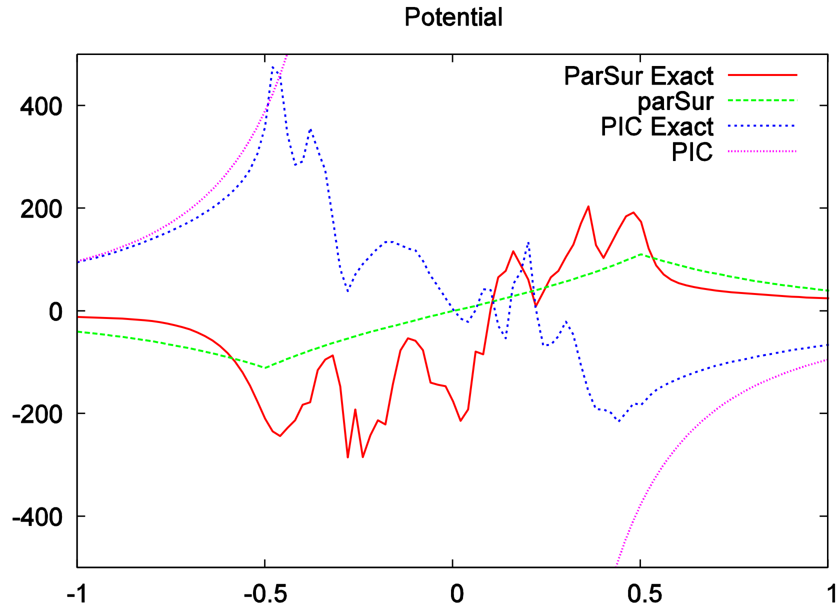
An improved model to represent space charge

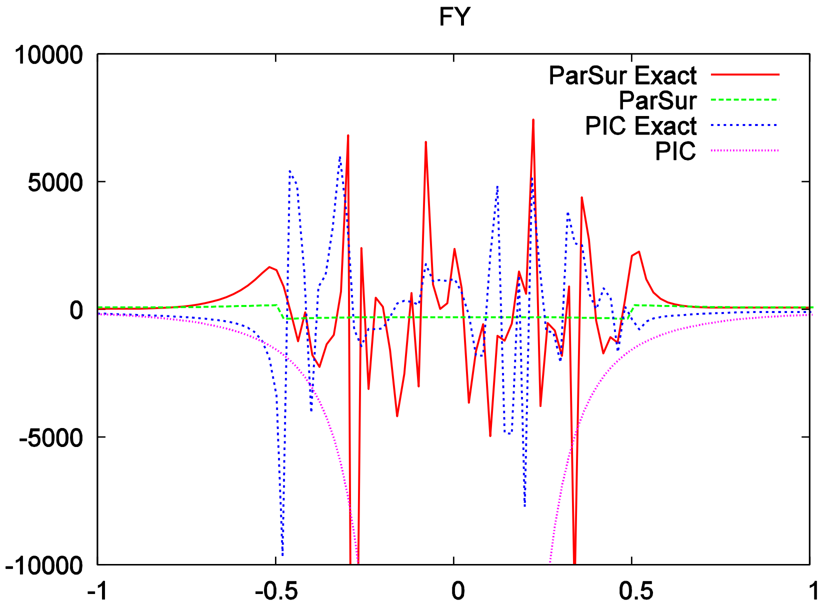


Possible only through the use of neBEM formalism

Space charge

Particles on Surface (ParSur)





- Although the results are preliminary, both potential and field within the cell has been estimated far more accurately by ParSur than PIC

PARticles on SURface (PARSUR) seems to be the new model to pursue!!

Adaptive Meshing

- Meshing (Delaunay) being worked upon using the CGAL library
- Arbitrary flat polygons have been discretized
- Complex shapes, such as holes, yet to be tried
- Needs lot more work
- Interface to be developed

Parallelization using multi-threading

Matrix size 10,000 × 10,000

Operation	Serial (seconds)	Parallel (seconds)
Influence matrix	27	5
Matrix decomposition	5313	1613
Column inversion	2303	1138
Solve	28	6
Total	7671	2762

Availability of multi-core CPUs on desktops and laptops

GPU computation will also be evaluated as an option

Future plan in Experiments

A small MPGD laboratory is being developed

Experimental efforts on:

Measurement of detector characteristics

Measurement of electric field distribution