The neBEM Field Solver and its possible application in the simulation of MPGDs

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MPGD (RD51) Workshop
April 16 – 18, 2008
NIKHEF, Amsterdam

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Outline of the presentation

- Relevance of a field solver in detailed MPGD simulation
- Brief introduction to Boundary Element Method
- Brief introduction to ISLES library and neEBM solver
- Validation of the closed-form exact expressions used
- Important numerical aspects
- Problem solving relevant to MPGDs
- Aspects to be implemented and final remarks

We will try to illustrate both numerical and application aspects

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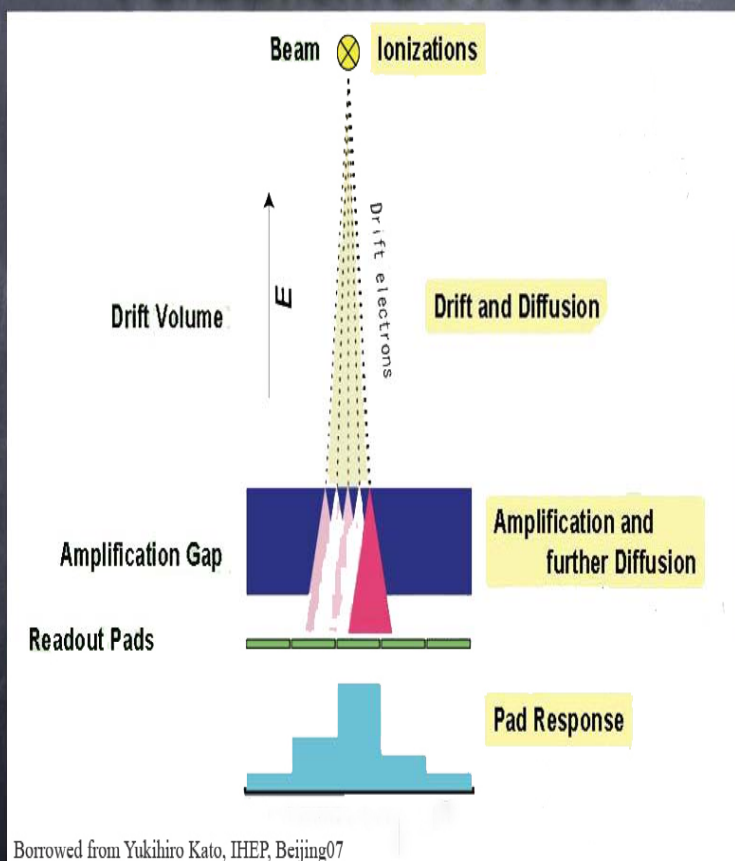S.Bhattacharya

A very brief tour
SINP, Kolkata, India

- An autonomous Institute under the Department of Atomic Energy, Government of India
- Named after the famous scientist Professor Meghnad Saha (Saha's Ionization equation)
- Small campus with around twenty divisions / sections belonging to ten groups / centers
- Approximately 125 students pursuing PhD, 150 faculties pursuing research and training, 300 supporting staff helping the Institute to carry on
- Kolkata, beside the Hooghly river, is charming during October – March. Moreover, both the Himalayas and the Bay of Bengal are quite close!

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The Field Solver is crucial at every stage
Isolated, at present

Fundamental Process

Beam ⊗ Ionizations

Drift Volume

E

Drift electrons

Drift and Diffusion

Amplification Gap

Amplification and further Diffusion

Readout Pads

Pad Response

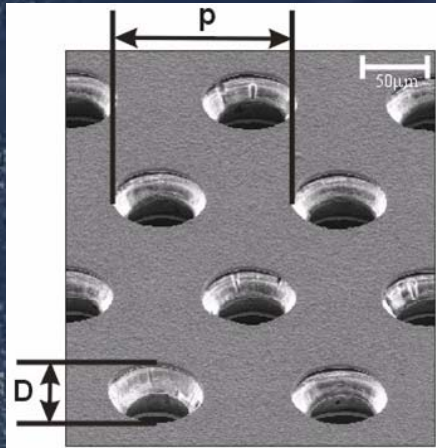Borrowed from Yukihiro Kato, IHEP, Beijing07

- 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**

Almost all the parameters depend on the local electro-static field. Thus, for modeling a dynamically changing system, a precise and efficient field solver should be integrated with all the other simulation components.
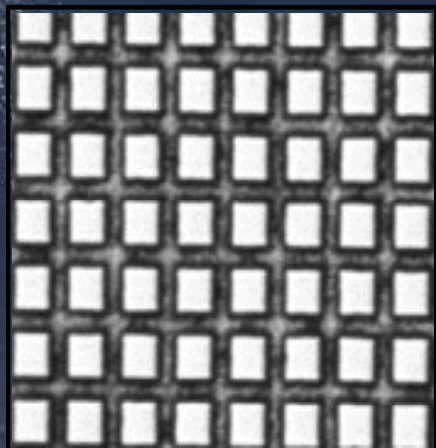
A Field Solver for MPGDs
Expected features

GEM Typical dimensions
Electrodes (5 µm thick)
Insulator (50 µm thick)
Hole size D ~ 60 µm
Pitch p ~ 140 µm
Induction gap: 1.0 mm,
Transfer gap: 1.5 mm

Micromegas dimensions
Mesh size: 50 µm
Micromesh sustained by
50 µm pillars

- Variation of field over length scales of a micron to a meter needs to be precisely estimated
- Fields at arbitrary locations should be available on demand
- Intricate geometrical features – essential to use triangular elements, if needed
- Multiple dielectric devices
- Nearly degenerate surfaces
- Space charge effects can be very significant
- Dynamic charging processes may be important
- It may be necessary to calculate field for the same geometry, but with different electric configuration, repeatedly

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A Solver of Laplace's / Poisson's equation

- Physical consequence of combining
  - ➢ A phenomenological law (inverse square laws, Fourier law in heat conduction, Darcy law in groundwater flow)
  - ➢ Conservation law (heat energy conservation, mass conservation)
- Primary variable, P; material constant, m; Source, S

$$\nabla.(m\nabla P) = S$$

Heat transfer: temperature, thermal conductivity, heat source
Electrostatics: potential, dielectric constant, charge density
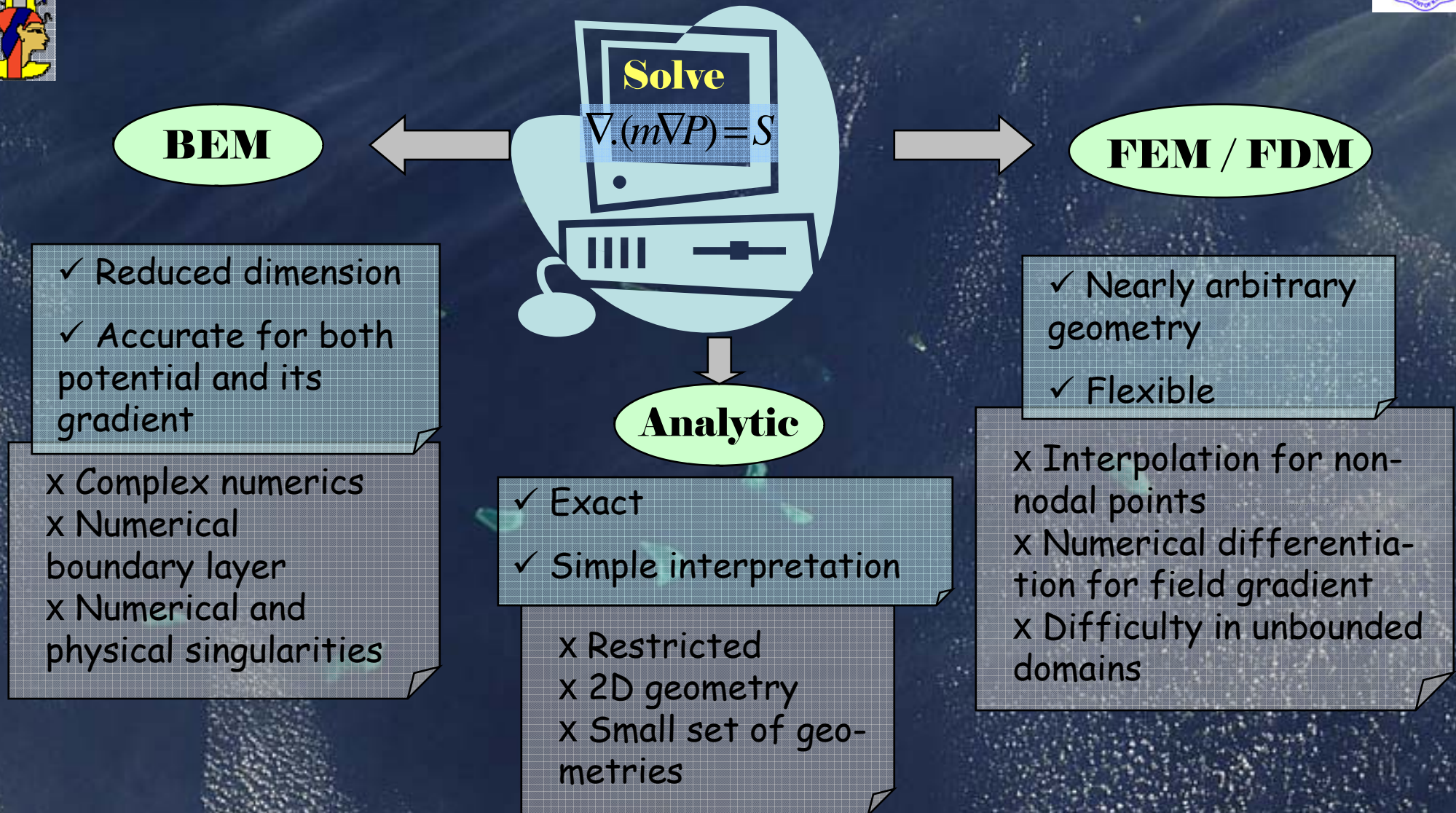Magnetostatics: potential, permeability, charge density
Groundwater flow: piezometric head, permeability, recharge
Ideal fluid flow: stream function, density, source
Torsion of members with constant cross-section: stress, shear modulus, angle of twist
Transverse deflection of elastic members: deflection, tension, transverse load
Many more …

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Solve

$$\nabla \cdot (m\nabla P) = S$$

BEM

FEM / FDM

Analytic

✓ Reduced dimension

✓ Accurate for both potential and its gradient

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

✓ Nearly arbitrary geometry

✓ Flexible

x Interpolation for non-nodal points
x Numerical differentiation for field gradient
x Difficulty in unbounded domains

✓ Exact

✓ Simple interpretation

x Restricted
x 2D geometry
x Small set of geo-metries

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FEM
the automatic choice?

- ✓ Handles arbitrary geometry using triangular surface / tetrahedral volume elements
- ✓ Multiple dielectric devices can be analyzed
- ✓ Sparse matrices are generated resulting into very efficient solution of the algebraic system of equations
- ✓ Very impressive array of commercial products that are well documented and benchmarked
- ✓ Huge user base

- ❖ Solves for potential at fixed nodal points distributed throughout the volume
- ❖ Variation of potential from node to node represented by low order polynomials
- ❖ Fields are, thus, represented by even lower-order polynomials
- ❖ Results at arbitrary points, not coinciding with nodes, can be inaccurate
- ❖ In regions of fast changing potential, and faster changing fields, estimates can oscillate and be unreliable.
- ❖ Geometrical features such as degenerate surfaces and extreme aspect ratios can be difficult to analyze
- ❖ Space charge modeling can be very difficult
- ❖ Repeated calculations can be very demanding in terms of computational resources
- ❖ Far-field needs to be truncated using artificial boundary conditions

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BEM
a possible candidate

- ✓ Solves for the charge density (or similar source / sink / doublet / vortex) on the device surface
- ✓ Both potential and field can be estimated using the charge density distribution – nominally exact
- ✓ Essentially Meshless – estimation of values at arbitrary locations in space is possible without necessitating interpolation / numerical differentiation
- ✓ Reduction of dimensionality – only the surface needs to be discretized
- ✓ Arbitrary geometries can be analyzed by using triangular elements
- ✓ Multiple dielectric devices can be studied
- ✓ Far field is naturally satisfied

- ❖ Relatively complicated mathematics
- ❖ Mathematical and physical singularities may occur
- ❖ Former can be removed by resorting complicated mathematics and adopting `special' formulations
- ❖ The latter results into the infamous numerical boundary layer leading to unreliable near-field estimates
- ❖ Densely populated matrices – some new and promising algorithms exist, though
- ❖ Space charge problems can be difficult to model
- ❖ Less availability of commercial packages
- ❖ Smaller user base

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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

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

$\alpha = 1$ 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 ↦ 0, r≠ 0
ln(r)	1/r	Weak singularity	Nearly weak singularity
1/r	1/r²	Strong singularity	Nearly strong singularity
1/r²	1/r³	Hyper singularity	Nearly hyper-singularity

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Solution of 3D Poisson's Equation
using BEM

- 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.

Electrostatics BIE

Potential at r

Charge density at r'

$$\Phi(\vec{r}) = \int_S G(r, \vec{r'}) \rho(\vec{r'}) dS'$$

Green's function

$$G(\vec{r}, \vec{r'}) = \frac{1}{4\pi\varepsilon \left| \vec{r} - \vec{r'} \right|}$$

ε - permittivity of medium

discretization

$$[A]\{\rho\} = \{\Phi\}$$

Influence Coefficient Matrix

$$\{\rho\} = [A]^{-1}\{\Phi\}$$

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.

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Conventional BEM

Major Approximations

Constant element approach

- While computing the influences of the singularities, the 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.

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

Mathematical singularities can be removed: Sufficient to satisfy the boundary conditions at centroids of the elements.

Difficulties in modeling physical singularities

geometric singularity

boundary condition singularity

Numerical boundary layer

Present Approach

Analytic expressions of potential and force field at any arbitrary location due to a uniform distribution of source on flat *rectangular* and *triangular* elements. Using these two types of elements, surfaces of any 3D geometry can be discretized.

Restatement of the approximations
- 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, modeled by the shape functions

ISLES library and neBEM Solver

Foundation expressions are analytic and valid for the complete physical domain

Contrast of approaches
nodal versus distributed

Influence of a flat triangular element in Usual BEM
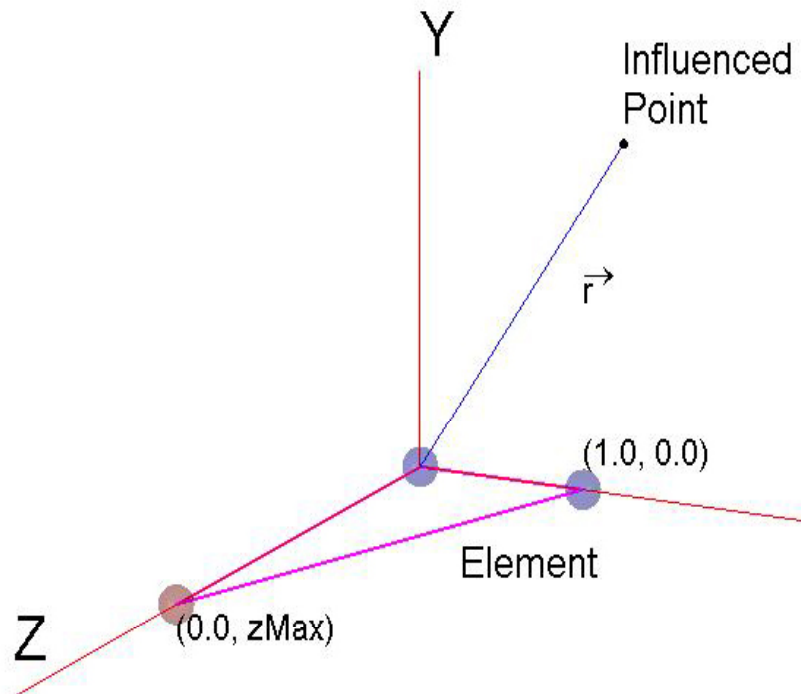
Influence of a flat triangular element in ISLES

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Foundation expressions of ISLES
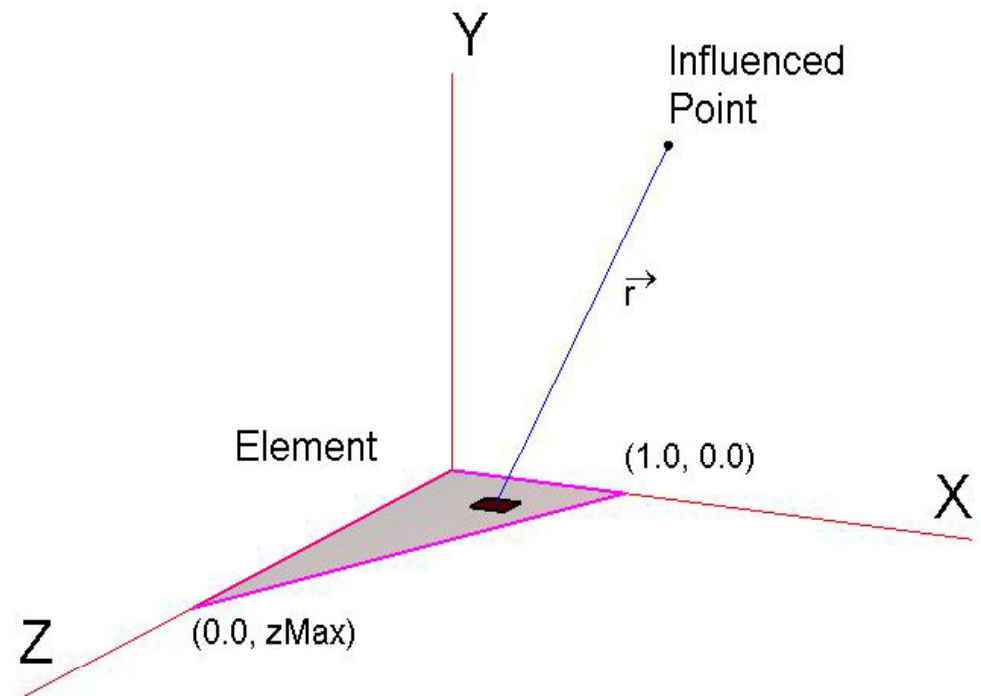
Inverse Square Law Exact Solutions

Rectangular elements

Influence of a flat boundary element

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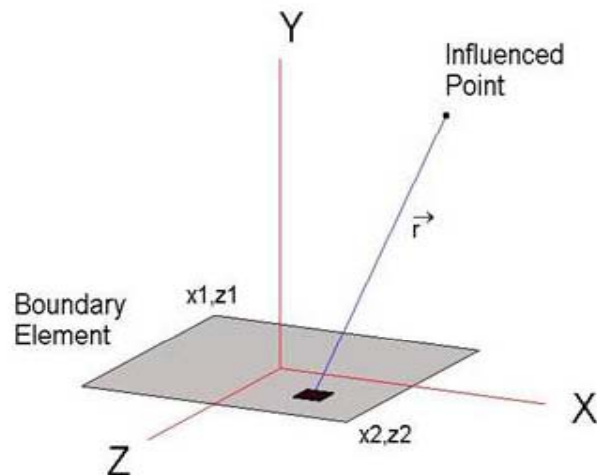
$$\frac{1}{2} \times \left\{ \begin{array}{l} 2 \times (X \mid Z \mid x_i \mid z_j) \times \ln\left(\dfrac{D_{i,j} - (X \mid Z - x_i \mid z_j)}{D_{m,n} - (X \mid Z - x_m \mid z_n)} \right) \\[2em] + iS_j|Y| \times \left[\tanh^{-1}\left(\dfrac{R_j - iI_i}{D_{i,j}|Z - z_j|} \right) - \tanh^{-1}\left(\dfrac{R_j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

4 log terms

4+4 complex tanh⁻¹ terms

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

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

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

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

$$\Phi(X,Y,Z) = \int_{x1}^{x2}\int_{z1}^{z2} \frac{dxdz}{\sqrt{(X-x)^2 + (Y-y)^2 + (Z-z)^2}}$$

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

May need translation and vector rotation

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

2 terms

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

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

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:

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

Potential distribution on the element

Validation

Force field in the Y direction

Force field in the Z direction

Validation

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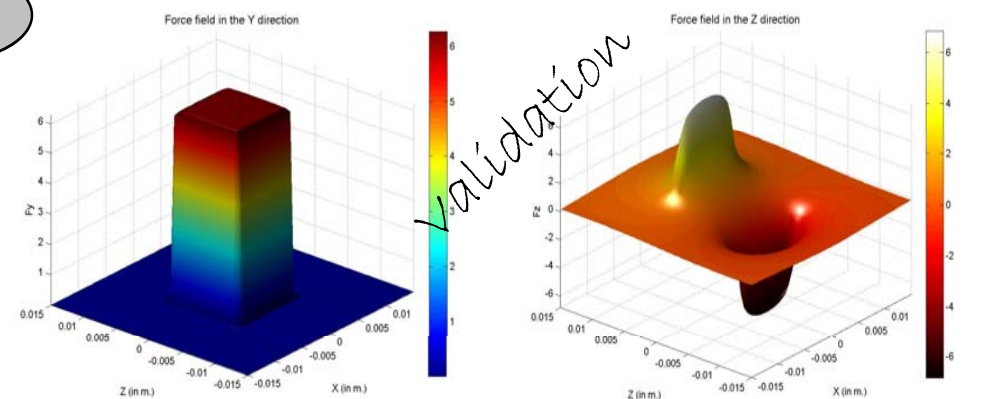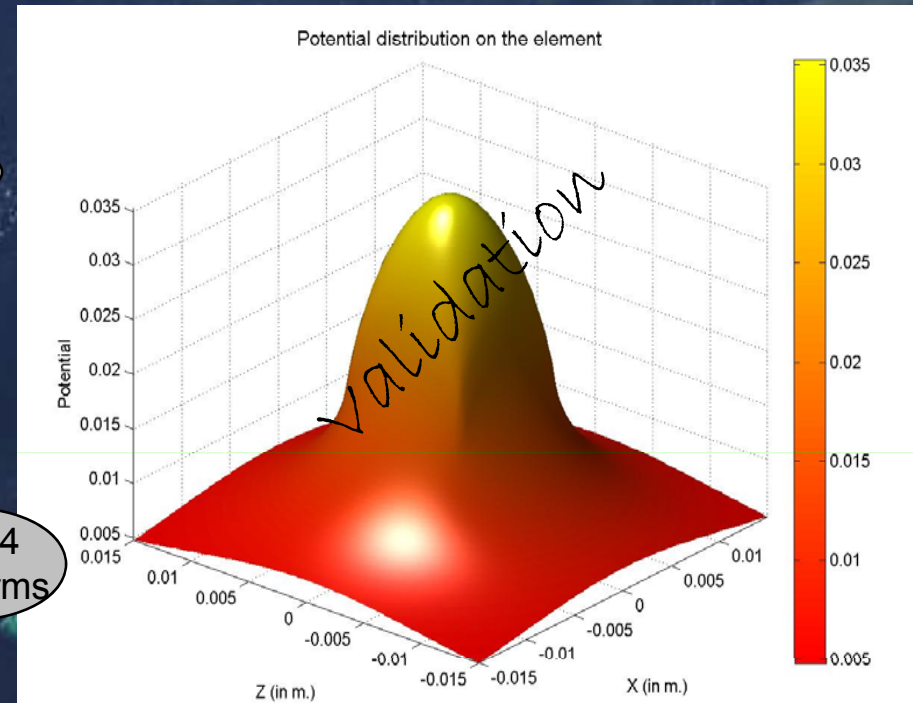
Foundation expressions of ISLES
Triangular elements

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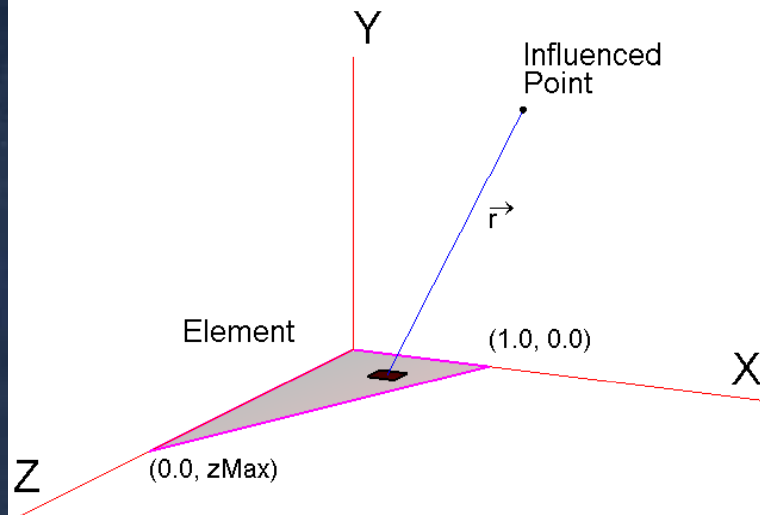
$$\Phi(X,Y,Z) = \int_0^1 \int_0^{z(x)} \frac{dxdz}{\sqrt{(X-x)^2 + (Y-y)^2 + (Z-z)^2}}$$

- 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 and triangular elements
- Evaluation of speed has been carried out using the Linux / UNIX system routine "gprof"

Similar expressions as for rectangular elements but much longer

May need translation, vector rotation and simple scalar scaling

Precision in flux computation

comparison with quadrature

zMax = 10.0
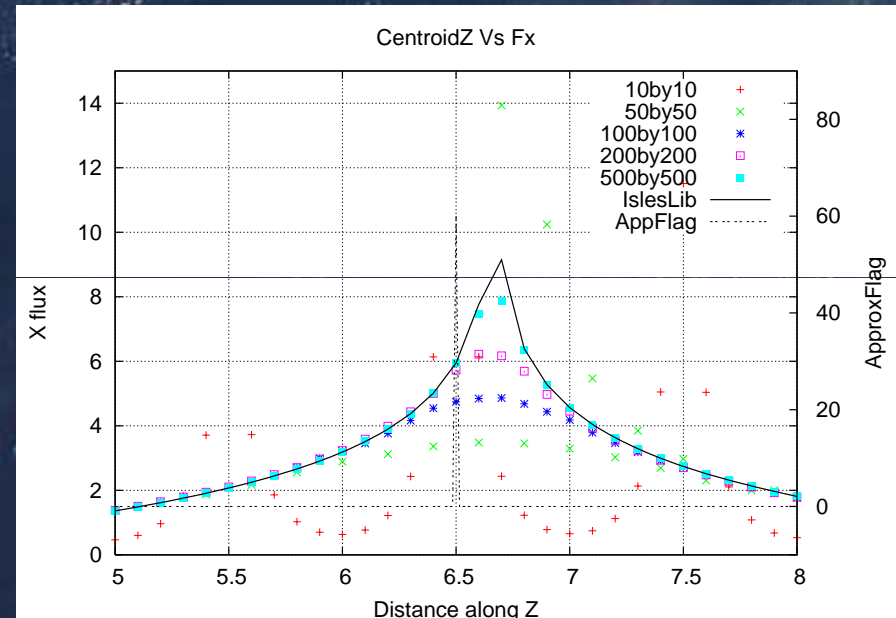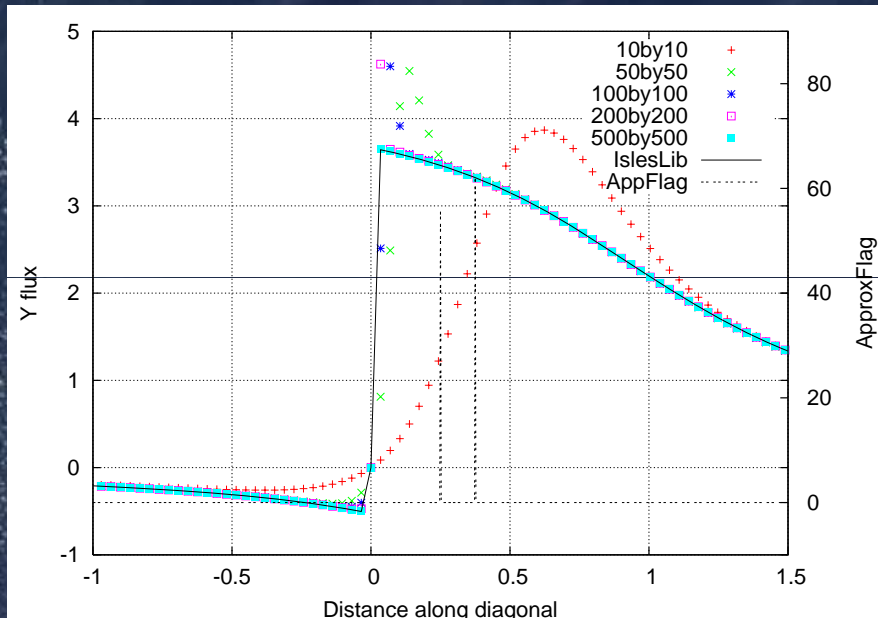
Quadrature with only the highest discretization produces results comparable to ISLES

Quadrature with even the highest discretization fails!

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Precision in flux computation
Comparison with multipole expansions
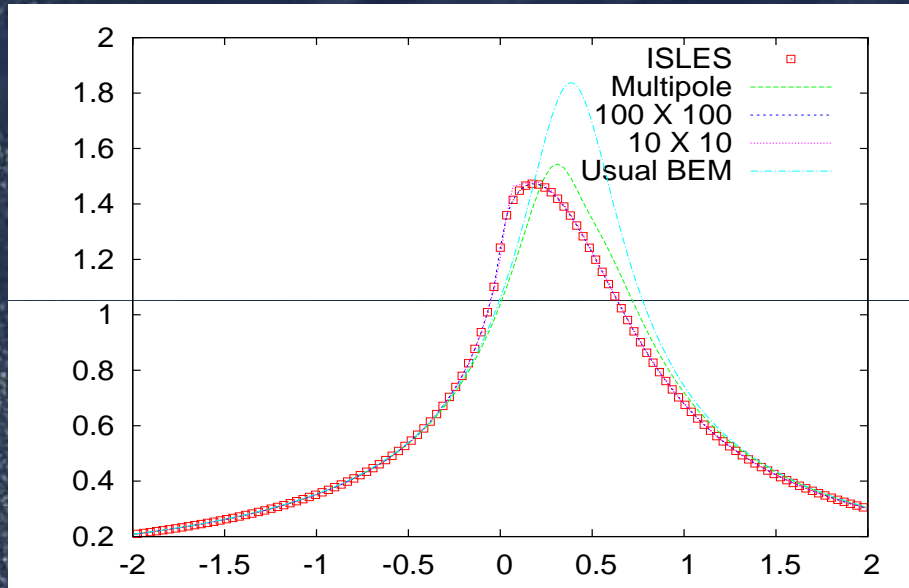
Comparison of flux along a line parallel
to the Z axis passing through the
barycenter
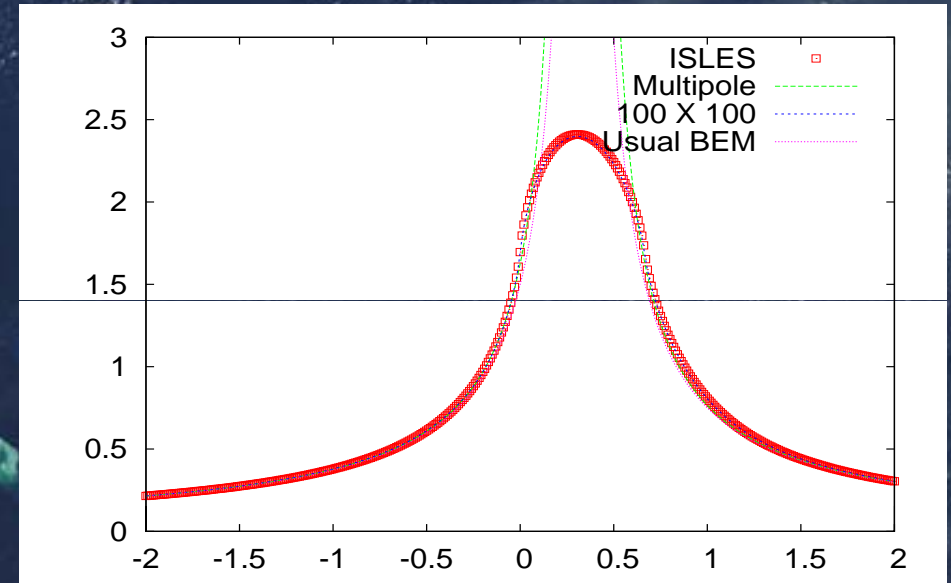
Comparison of flux along a diagonal
passing through the barycenter

The quadrupole results are still far from precise

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Need for Speed!

- We carried out a small performance analysis
- Following table reflects the initial information which seems to be quite encouraging …

Element	Evaluation	Time	Element	Evaluation	Time
Rectangular	Exact	0.6 µs	Triangular	Exact	0.8 µs
Rectangular	1 by 1	25 ns	Triangular	100 by 100	200 µs
Rectangular	10 by 10	2 µs	Triangular	500 by 500	5 ms

✓ So, for a prescribed accuracy, the gain in speed is enormous
✓ This is especially true if near field computations are of interest

Need for Speed
A closer study on errors
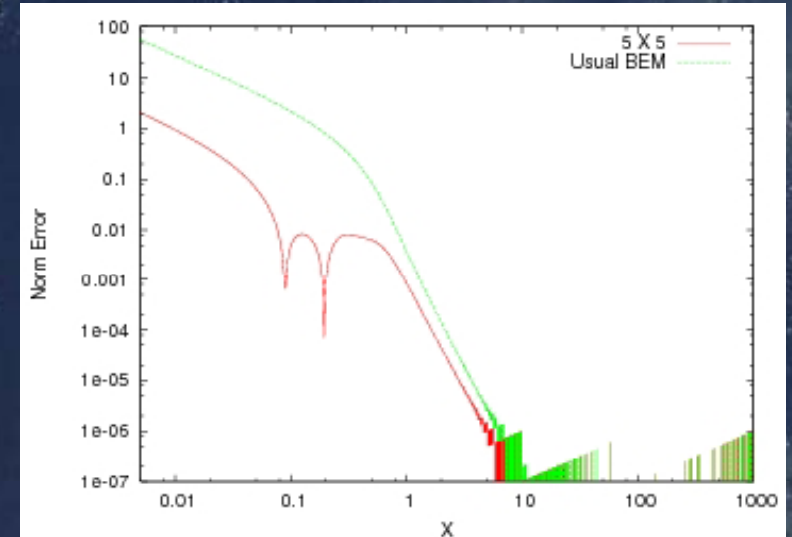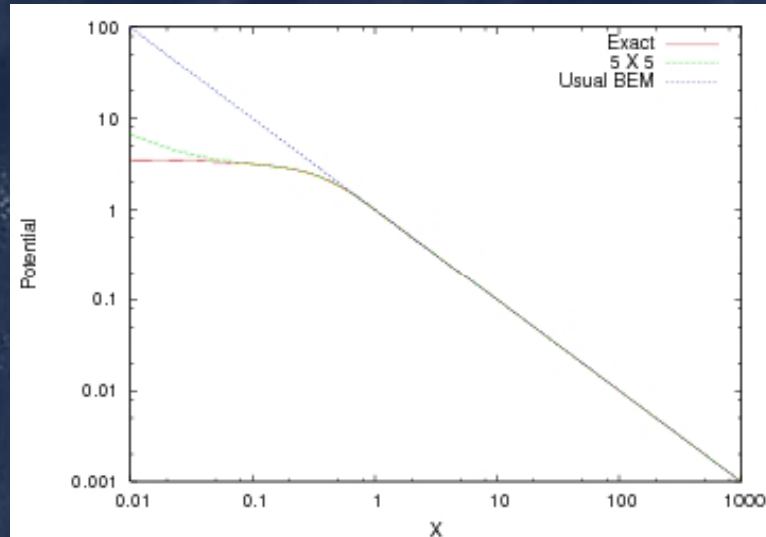
- Along diagonals, 5 by 5 discretization produces error less than 1% beyond 1 unit

- Along axes, the errors is less than 1% only if the distance is 3 units or more

- For far-field points (> 5 units), usual BEM should be used to minimize computational expenses

Precision and Speed

a detour on important numerical aspects

- To err is computational, unfortunately
  - ➤ Presence of singularities
  - ➤ Round-off errors
  - ➤ *NaN, inf*

- Approximation flags – a temporary measure!

- Other Issues
  - ➤ Transcendental functions
  - ➤ Multi-valued functions
  - ➤ Complex vs. real functions

Away from the realm of mathematics
Requirements for MPGDs

- A new set of closed-form exact solutions for precise estimation of potential and flux due to singularities (sources, sinks, doublets etc) uniformly distributed over rectangular and triangular elements has been found. These have evolved into a C library, namely ISLES

- Based on this library, the neBEM (nearly exact Boundary Element Method) solver has been developed to solve problems of interest in science and engineering

- Since Poisson's equation is one of the most important one in classical physics (an integral expression of the inverse square law and the laws of conservation) governing much of gravitation, electromagnetics, structural mechanics, ideal fluid mechanics, Stoke's flow, acoustics, optics and so on, these solutions can have vast applications.

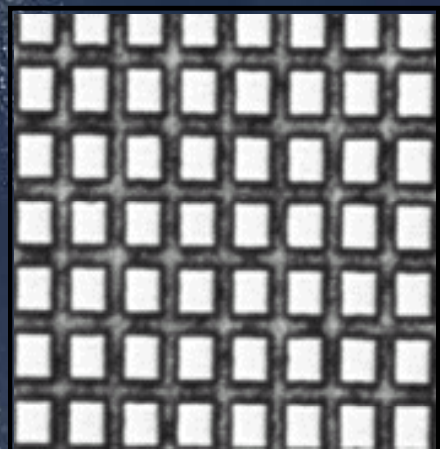- But what about problems related to MPGD simulation?

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Review

Expected features of A Field Solver for MPGDs

GEM Typical dimensions
Electrodes (5 μm thick)
Insulator (50 μm thick)
Hole size D ~ 60 μm
Pitch p ~ 140 μm
Induction gap: 1.0 mm,
Transfer gap: 1.5 mm

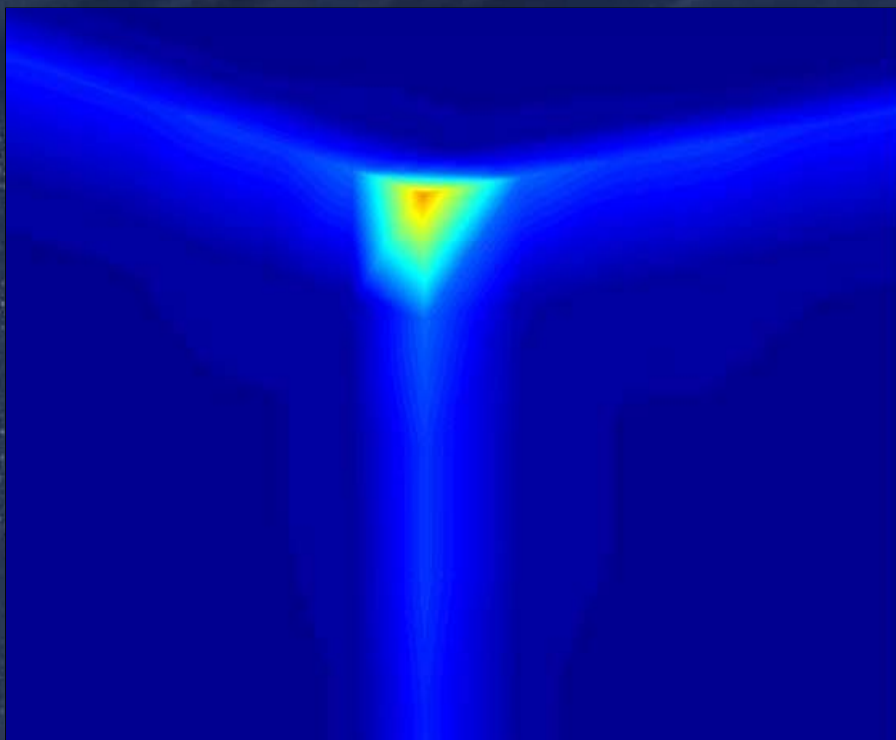

Micromegas dimensions
Mesh size: 50 μm
Micromesh sustained by
50 μm pillars

- Variation of field over length scales of a micron to a meter needs to be precisely estimated
- Fields at arbitrary locations should be available on demand
- Intricate geometrical features – essential to use triangular elements, if needed
- Multiple dielectric devices
- Nearly degenerate surfaces
- Space charge effects can be very significant
- Dynamic charging processes may be important
- It may be necessary to calculate field for the same geometry, but with different electric configuration, repeatedly

Length scales
A micron in a meter

One of the major unsolved problems of electrostatics – A unit conducting cube raised to unit volt

X	Y	Z	NIMA **519** Potential	neBEM Potential
0	0	0	0.999990	1.000001
0.4	0.5	0.5	0.9996	0.9994362
0.45	0.5	0.5	0.99986	0.9995018
0.49	0.5	0.5	1.0013	0.9991151
0.499	0.5	0.5	1.0048	0.9987600
0.4999	0.5	0.5	-	0.9974398
0.49999	0.5	0.5	-	0.995135
0.499999	0.5	0.5	-	0.9945964

Charge density distribution at one of the corners

Arbitrary locations
Very close to the wire of an Iarocci tube
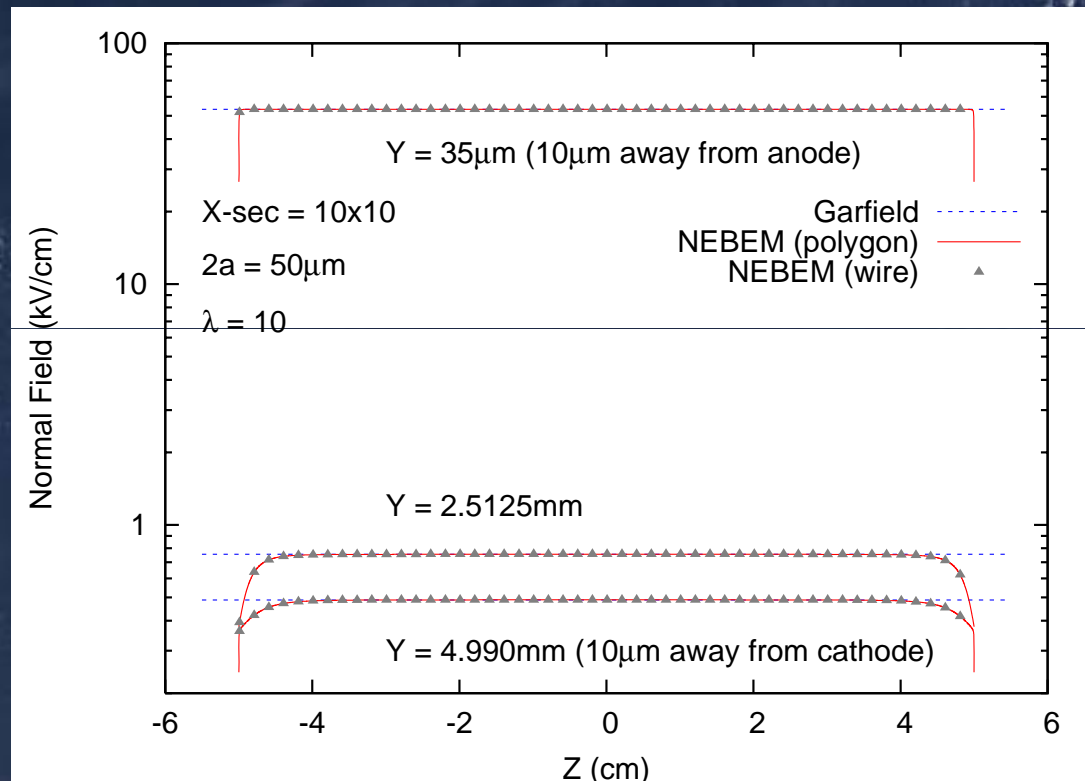
Axial deviation of normal electric field at the mid-plane of an Iarocci chamber with cross-section 10mm × 10mm.

Two different models of wire have been considered

> ➤ Despite the proximity of the top line to the wire surface, the normal electric field is found to be completely free from jaggedness or oscillations
> ➤ Unfortunately, we do not have FEM packages (they are expensive!). Hence, it has not been possible for us to compare results on this case

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Intricate geometries

The Micro Wire Detector
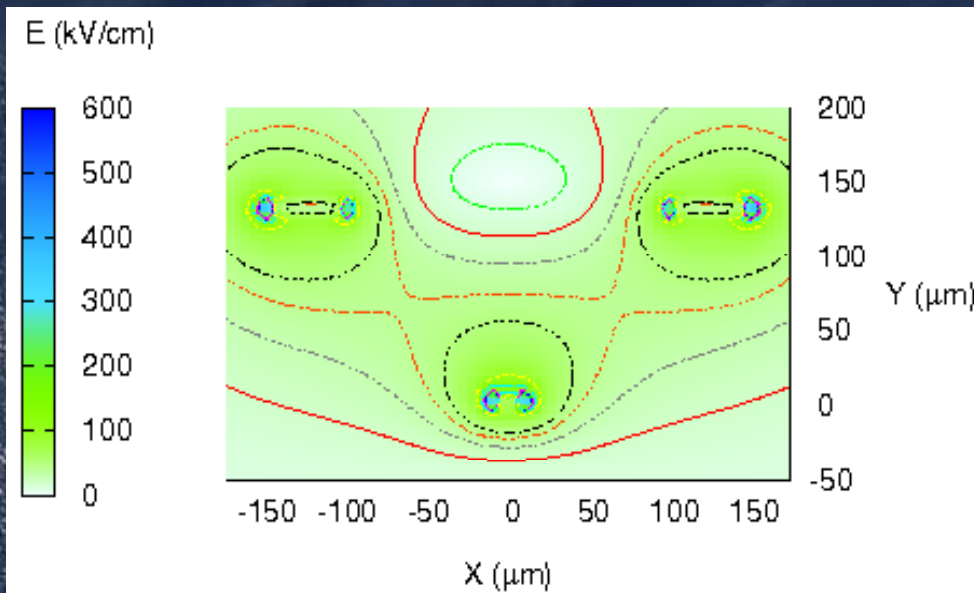
Total electric field contours on the central plane across cathode and anode
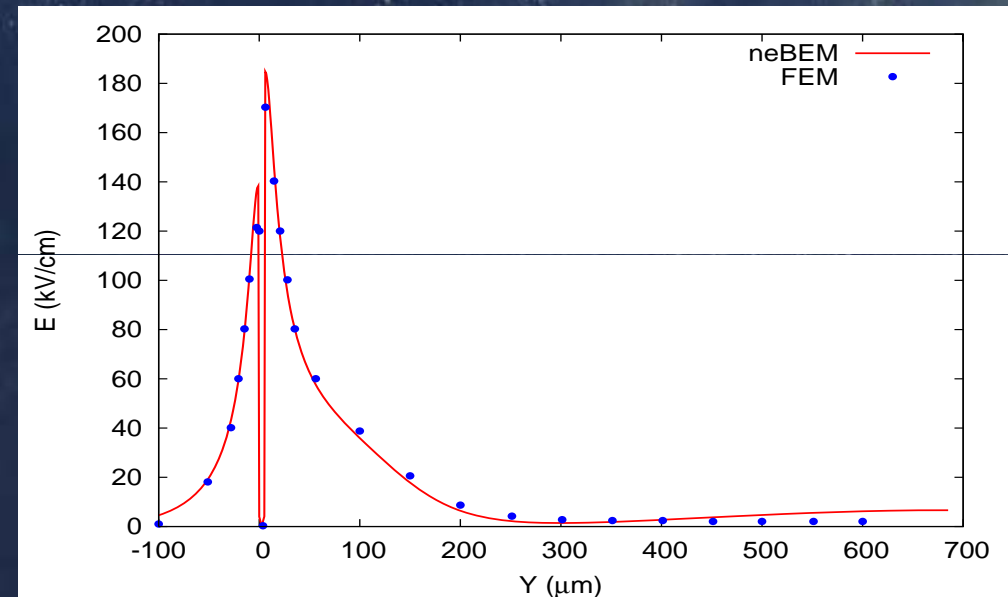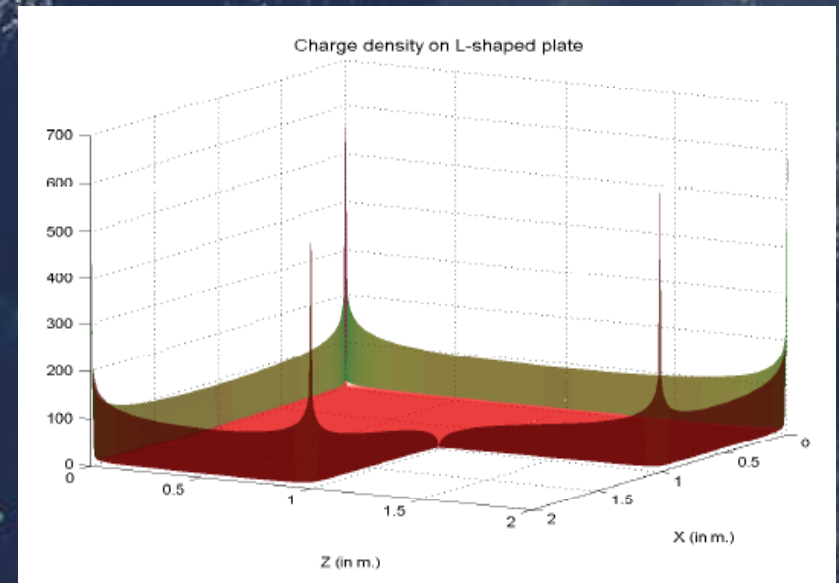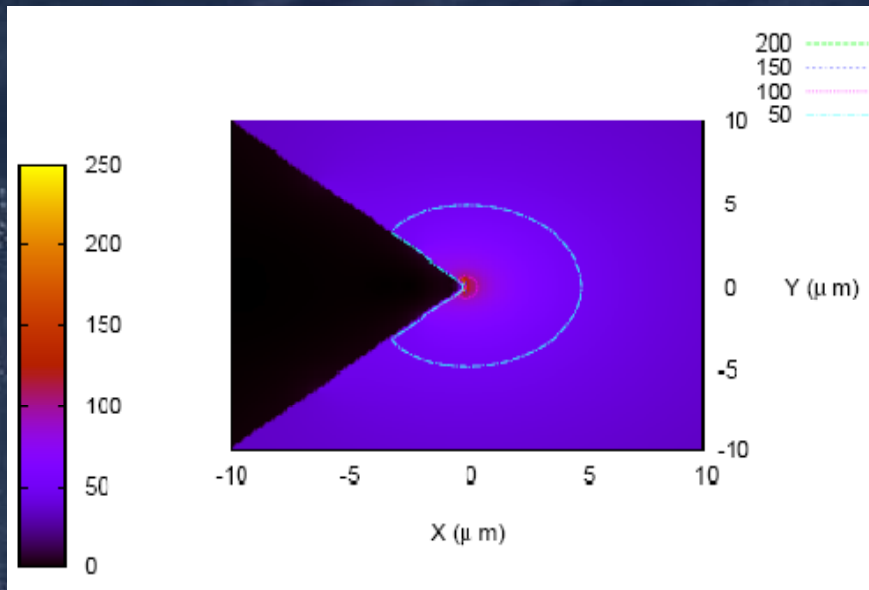

Variation of total electric field along an axis passing through the mesh hole

➢ The MWD has an intricate design. In this case: Drift plane 785µm from the anode strip at 1.11kV.

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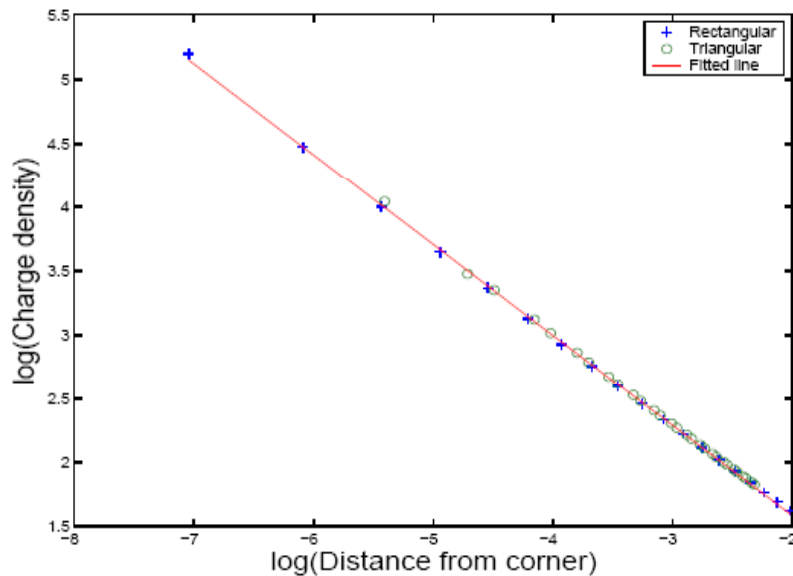S.Bhattacharya

Intricate geometries
sharp corners

➢ Electrostatics of both inner and outer corners have been estimated
➢ It has been possible to estimate field to within 5% for a point within a micron of a convex corner
➢ For a concave corner, usable estimation could be made upto within 10 microns of 90° corner

Triangular element
## *Corner charge density of a unit square plate*

Method	Order of singularity
Numerical shooting	0.7034
Walk on spheres	0.7034
Surface charge	0.704
Ficehra's theorem	0.7015
Walk on plane	0.7034
neBEM	0.7057 (triangular) 0.7068 (rectangular)

Variation of charge density with Increasing distance from the corner

Multiple Dielectric
Complicated by the presence of degenerate surfaces

Multiple Dielectric Geometry
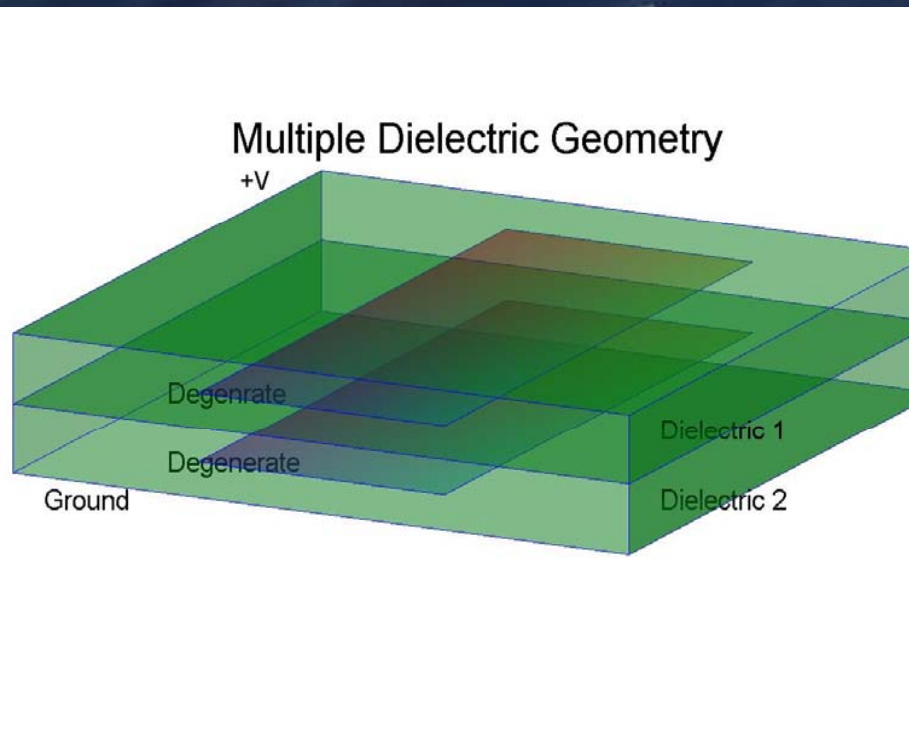
	Ratio of dielectrics = 10		
Location	FEM	DBEM	Present
24.0,16.5	0.514489	0.52181	0.5247903
6.5,12.0	0.2301575	0.23801	0.2398346
22.5,6.0	0.3638855	0.34638	0.3451232
4.0,3.5	0.1108643	0.10623	0.1058357

Please note that all the distances are in microns

Multiple dielectric
Resistive plate chambers
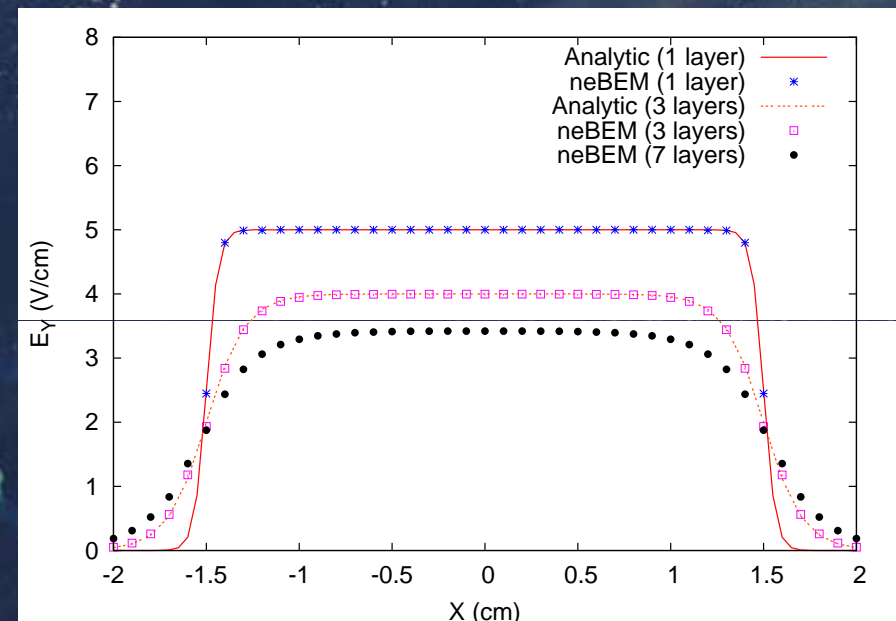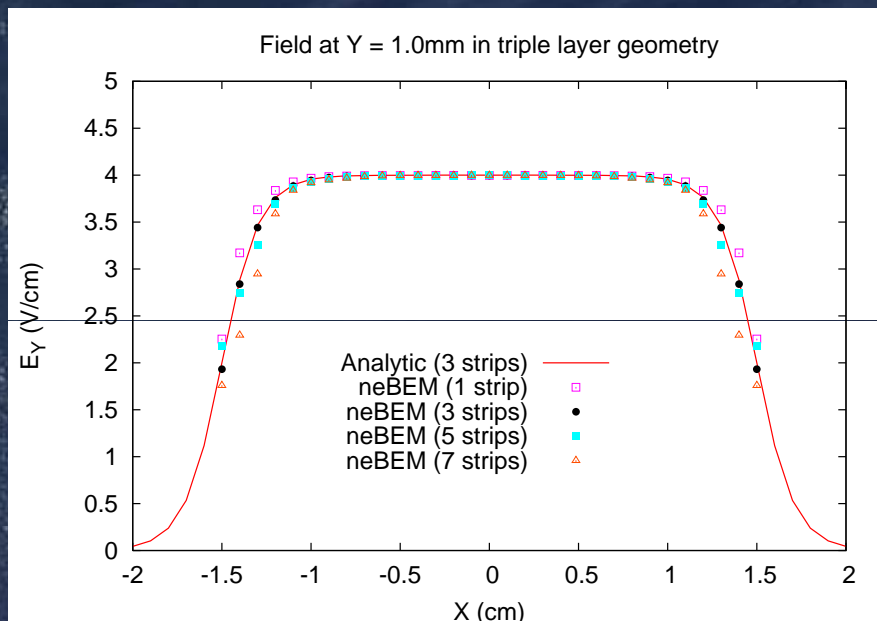
Strip width: 3.0cm, Strip length: 50.0cm
Layer height: 2.0mm
Layer-3 permittivity (ε_r): 7.75 (~glass)
Layer-2 (middle) permittivity (ε_r):
1.000513 (~Argon)
Successful validation with Riegler et al.

Layer-4,5 height: 200μm (~PET)
Layer-6,7 height: 20μm (~Graphite)
Layer-4,5 permittivity (ε_r): 3.0 (~PET)
Layer-6,7 permittivity (ε_r): 12.0 (~Graphite)

Nearly degenerate surfaces
Too many BEM formulations!

Geometry of the Model MEMS Structure
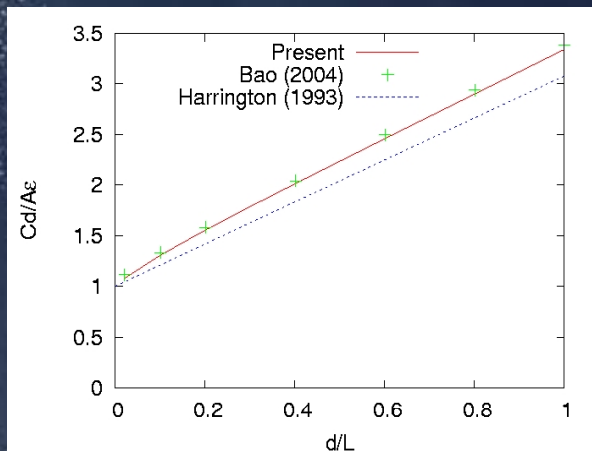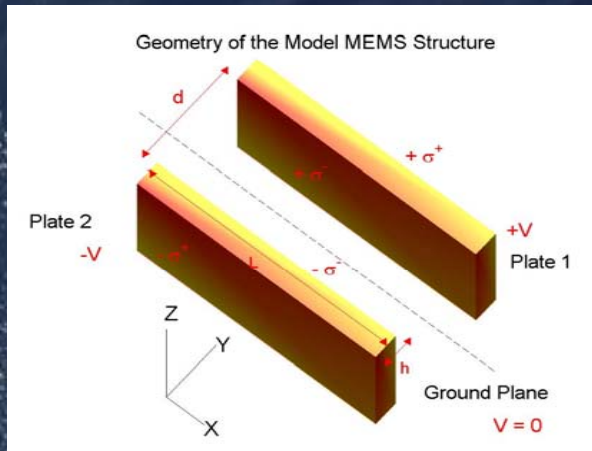
| h/L (for d/L 0.2)	Usual BEM	Enhanced BEM	Thin plate BEM	neBEM (- sides)	neBEM (+sides)
1.0	2.3975			1.259038	2.374961
0.1	3.3542	2.6631	1.2351	1.360813	1.757175
0.05		1.7405	1.3879	1.392805	1.679710
0.01		1.6899	1.5611	1.455047	1.590639
0.005		1.6652	1.5874	1.475206	1.574417
0.001		1.6221	1.6094	1.511291	1.558108
0.000001			1.6200 (1.5830)	1.539550	1.552190

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Repetitive estimations
Weighting field in RPC
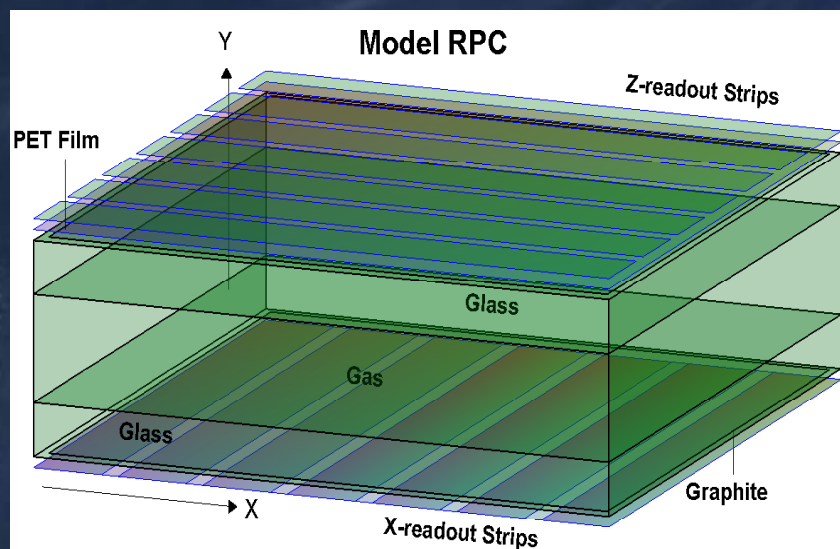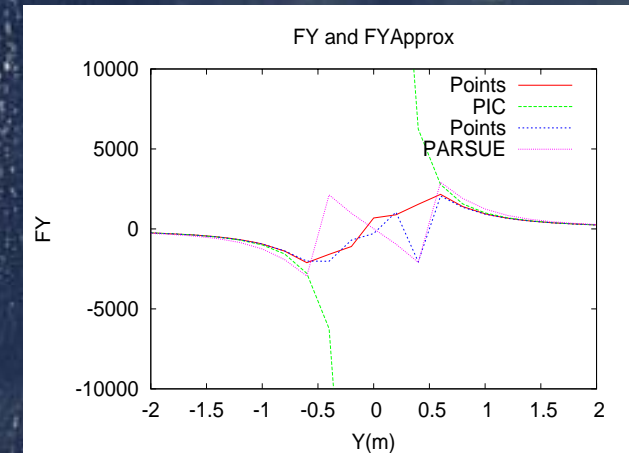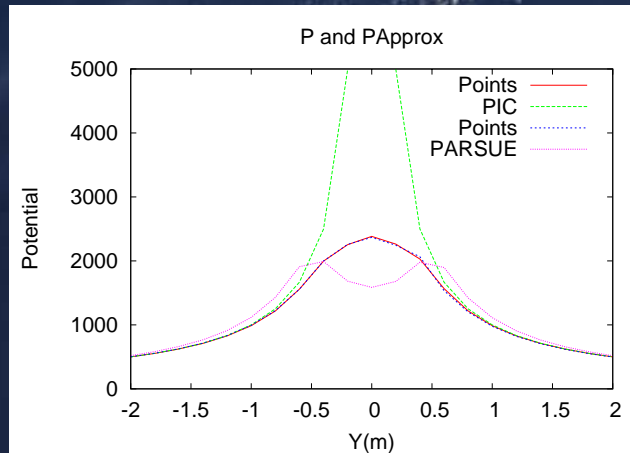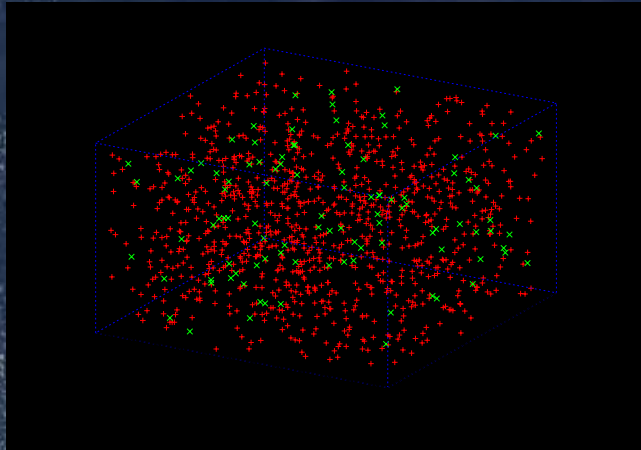

Schematic representation of the model RPC
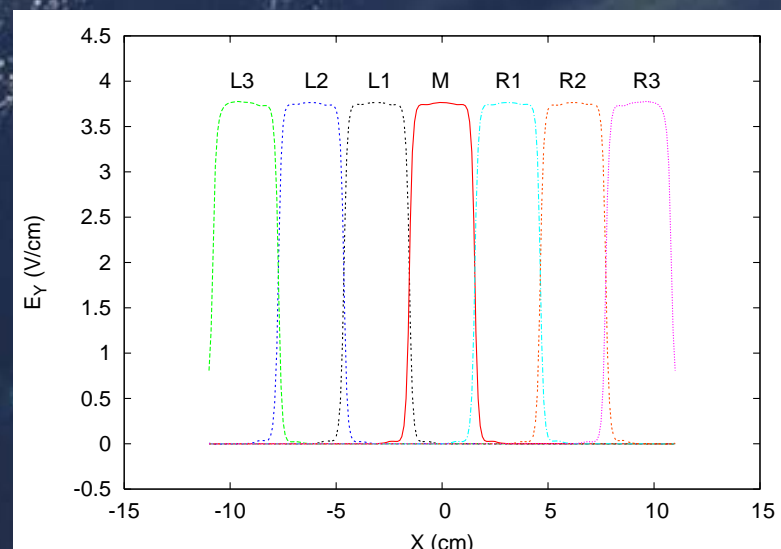
Plot of normal weighting field for all
The X-readout strips at the mid-section

➤ Note that, since the geometry of the problem remains unchanged, the influence coefficient matrix needs to be created and inverted only once.
➤ All the solutions involve just a matrix multiplication.

Space charge
Particles on Surface (ParSue)

- ❑ Create two sets of surfaces within the relevant volume placed perpendicular to the average direction of the negative and positive particles in a given avalanche
- ❑ Divide these surfaces into smaller elements
- ❑ Attach each positive and negative particle to its nearest surface element
- ❑ Compute the resulting surface charge density on each elemental surface
- ❑ The effect of the particle distribution can now be computed as the combined effect of these surface elements
- ❑ More precise and more efficient variants of ParSue are being explored

PARticles on SUrfacE (PARSUE) seems to be the new thing to pursue!!

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Gaps
and how to get rid of them

o The problem of dynamic charging has not been addressed.

o ParSue needs to be explored and integrated properly.

o Mesh generation has been implemented in a rather ad hoc manner; rigorous but user-friendly implementation is a necessity – should be related to the Geant4 approach, if possible.

o Minimum use of triangular elements (without losing on the precision front) needs to be ensured since the computation for triangular elements is considerably more than that for rectangular elements.

o Implementation of better algorithms to handle these huge and dense matrices can make wonders.

o Computational effort should be optimized – use of symmetry, adaptive mesh generation can help reducing the computational expenses by a significant amount

o Parallel computation can help the overall detailed simulation

o Interfaces to Garfield and ROOT needs to be developed to integrate neBEM into the detailed detector simulation and Geant4 frameworks.

Final remarks
A lot needs to be done in future

- A precise and efficient field solver, neBEM, based on the ISELS library, has been introduced
- It already has most of the major features necessary to carry out detailed MPGD simulation, including capability of simulating space charge
- Improvements necessary to make it more appropriate to the detailed detector simulation framework seems straight-forward but is likely to take some time
- It can be easily provided as a toolkit to the developer / user so that, in addition to detailed detector simulation, it can be used for Geant4 and other simulation studies.

Acknowledgements

➢ Organizers
- ❑ For inviting me to present this work in the workshop and join the collaboration meetings

➢ Director, SINP
- ❑ For supporting us throughout the course of the work and promising further support

➢ Rob Veenhof
- ❑ For his valuable remarks and suggestions

➢ And so many others who have encouraged, helped …

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The neBEM Field Solver for MPGDs

Thank you all!