Boundary Element Method

RD51 Lectures

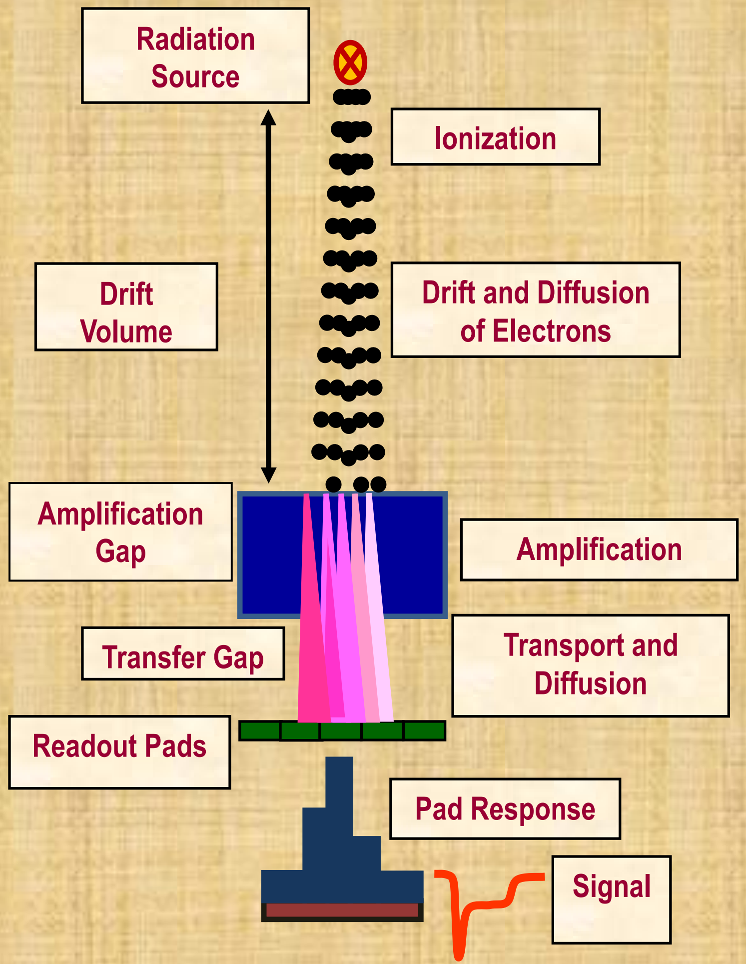
RD51 Collaboration Meeting, 22-26 June 2020

Outline

- Motivation
- Brief discussion on numerical modeling and options available for solving problems related to electrostatics
- A whirlwind tour of the integral approach, Green's function and Boundary Integral Equation
- Boundary Element Method, different formulations of the BEM, compare single point collocation and nearly exact BEM (neBEM)
- Validation and applications of neBEM
- Present status, future plan of neBEM
- Summary

Some of the slides are for later studies.
They will be touched upon briefly during the lecture.

Detector and its simulation

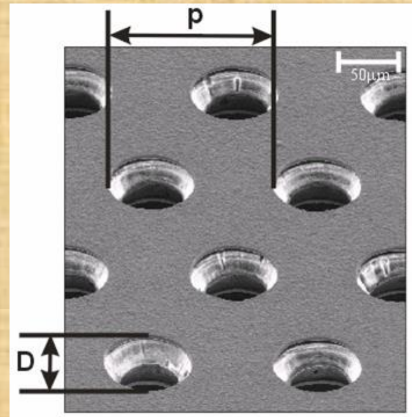


Simulation steps

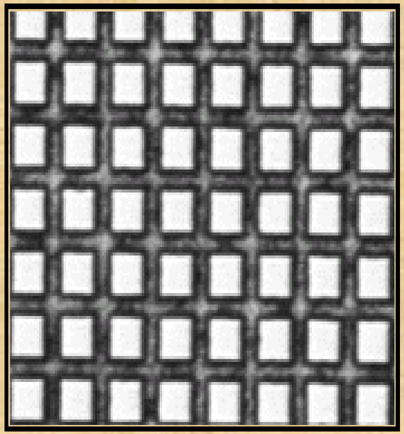
- **(1) Ionization:** energy loss through ionization of a particle crossing the gas and production of clusters – **HEED / MIP**
- **(2) Transport and Amplification:** electron drift velocity and the longitudinal and transverse diffusion coefficients - **MAGBOLTZ**
- **(3) Detector Response:** charge induction using reciprocity theorem (Shockley-Ramo's theorem), particle drift, charge sharing (pad response function - PRF); charge Collection – **GARFIELD / GARFIELD++**
- **Signal generation and acquisition: SPICE**
- **Electromagnetic field:** except ionization, each step depends critically on physical / weighting electric field and magnetic field, if present (**Analytic / ANSYS / COMSOL / neBEM / Elmer-Gmsh etc**).

Field solving is especially critical for MPGDs, due to their intricate, essentially 3D geometry.

Field Solver for MPGDs



GEM
Typical dimensions:
Electrodes: ~5 μm
Insulator: ~50 μm
Hole size(D): ~60 μm
Pitch(p): ~ 140 μm



Micromegas
Typical dimensions:
Mesh size: 50 μm
Micromesh sustained by pillars of 200 μm diameter

Expected features

1. Handle large variation in length scales (a micron to a meter)
2. Make available, on demand, properties at arbitrary locations (near- and far-field)
3. Model intricate geometrical features using triangular elements as and when needed
4. Model multiple dielectric devices
5. Model nearly degenerate (closely packed) surfaces
6. Model space charge effects
7. Model dynamic charging processes
8. Compute field for the same geometry, but with different electric configuration, repeatedly

- The de-facto standard FEM is unsatisfactory in dealing with 1., 2., 5., 6. and 7.
- Hence, the search for a new tool.

Reality ⟹ Model

Reality

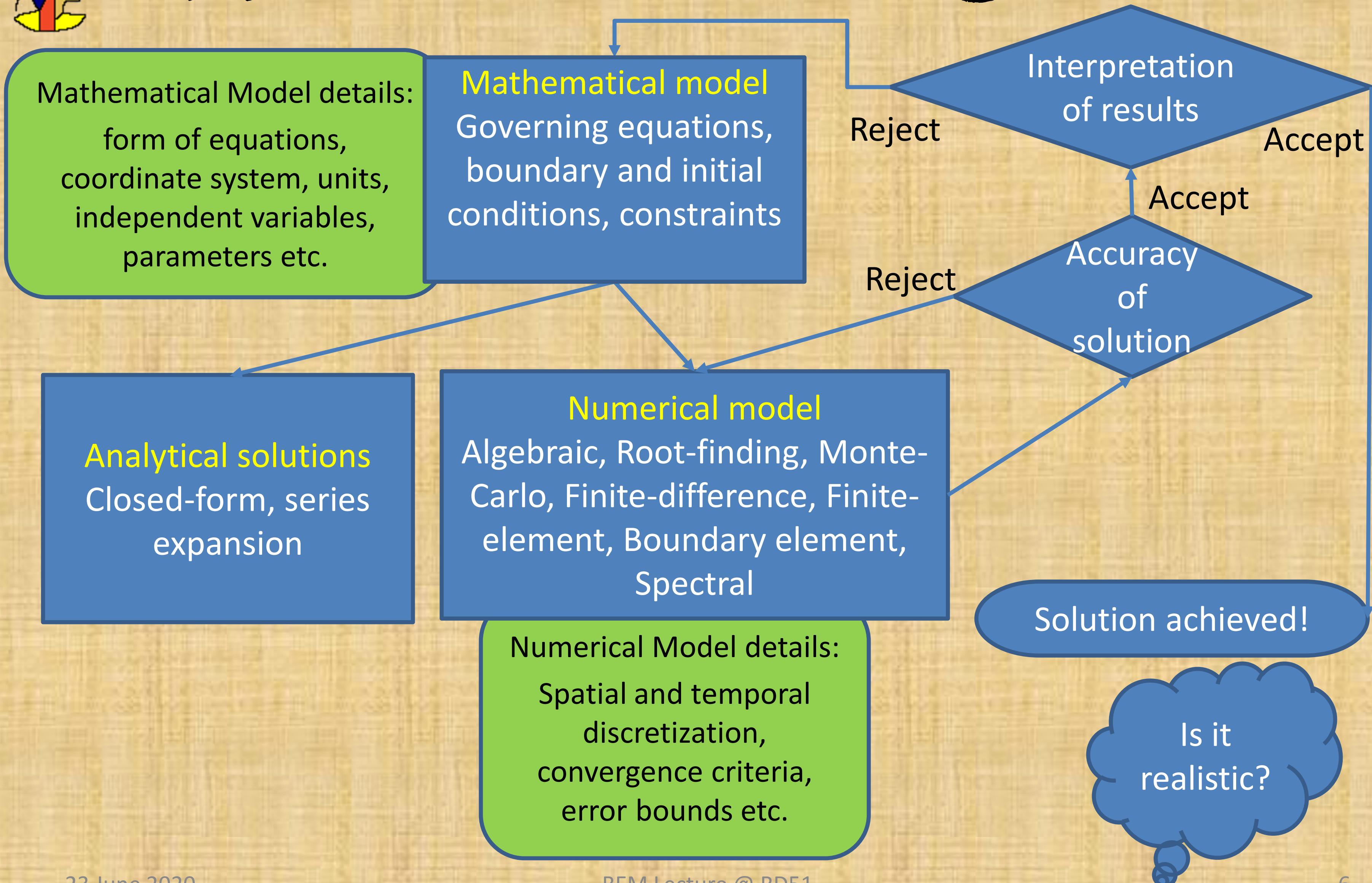
Physical theory
electromagnetism,
classical mechanics,
nuclear physics

Theoretical assumptions:
static, harmonic, transient,
2D, 3D, axisymmetric, linear,
non-linear

Mathematical model
Governing equations,
boundary and initial
conditions, constraints

Mathematical Model details:
form of equations,
coordinate system, units,
independent variables,
parameters etc

Mathematical model ⇨ Solution



Physics theory of field ->Mathematical model

Laplace's / Poisson's equation

- Mathematical consequence of combining
  - A phenomenological law (inverse square laws, Fourier law in heat conduction, Darcy law in groundwater flow)
  - Conservation law (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 …

Mathematical model -> Solution

Solve

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

BEM

- ✓ Reduced dimension
- ✓ Accurate for both potential and its gradient

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

Analytic

- ✓ Exact
- ✓ Simple interpretation

- x Restricted
- x 2D / axisymmetric geometry
- x Small set of geometries

FEM / FDM

- ✓ Nearly arbitrary geometry
- ✓ Flexible

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

The best in the world!

- Analytic solutions are exact.
- Precise values are obtained and it is relatively easy to evaluate parameter dependence.
- A *closed form solution* is one in the form of an explicit, algebraic equation in which values of the problem parameters can be substituted.
- Most analytic solutions are obtained assuming certain simplifications, thereby making the solutions applicable to those idealized situations.

The real, complex world!

- Complexity of the real-world leads to complex mathematical models.
  - Differential equations (ordinary and partial), integral equations, integro-differential equations
  - There can be a system of such equations
  - They can be non-linear and strongly coupled
- Analytic solution of these models are usually not available.
- Numerical methods are usually the only way out.
- Please note that the same problem can often be represented by both differential equations and integral equations.

Solution approach

- Starting point:
  - Governing equation (for us, it is the Poisson's equation)
    - elliptic PDE / equivalent integral equation
  - Computational domain
  - Boundary and / or initial conditions
- Method:
  - Discretize space into a finite number of sub-regions / elements,
  - Derive governing equation for a typical node / element (can be nodal, surface, or volume element),
  - Assemble all elements in the computational domain,
  - Solve the system of algebraic equations

Numerical methods

- Domain dividing (differential equation) methods and boundary dividing (integral equation) methods
- For domain methods, the unknowns are usually potentials.
  - Finite-difference: nodes throughout domain; Finite-volume: volumes throughout domain; Finite-element: elements throughout domain; Monte-Carlo: various possibilities
- For integral methods, the unknowns are usually charges / charge densities.
  - Charge simulation: fictitious charges inside conductors and dielectrics; Surface charge and Boundary element: charges on elements on interfaces of conductors and dielectrics

Note that there is significant variation in nomenclature, especially for the latter group

Comparison of principal numerical methods for electric fields

	Domain-dividing methods		Boundary-dividing method	
	FDM	FEM	CSM	SCM, BEM
Unknowns	Potentials at lattice (grid) points	Potentials at nodes	Fictitious charges	Charge densities for SCM, potentials and field strengths for BEM
Max. number of unknowns	$\approx 10^7$		$\approx 5 \times 10^4$	
Coefficient matrix[a]	Sparse		Full or dense	
How to obtain field values	(Potential difference)/distance or numerical differentiation of potentials		Analytical expressions for fields caused by charges	Numerical integral of fields caused by charge densities (or analytical expressions for planar charges)
Applicability and other features	Applicable to any problem, including nonlinear cases	Applicable to any problem, including nonlinear cases	Applicable to Laplacian fields, in particular, suitable for 2D and AS conditions	Applicable mainly to Laplacian fields, but more general than CSM
	Easy to subdivide domains Difficult to handle complicated or curved boundaries	More flexible than FDM, but more complicated programming and input data Suitable for complex, intricate problems	Needs experience and intuition to adopt proper positions of charges and contour points Difficult to deal with thin materials	Often troublesome in numerical integration when a computation point coincides with a source (charge)

Indirect BEM solves for charges!

Ref: Electric fields in Composite Dielectrics and their applications, Takuma and Techaumnat, Springer, 2010

Brief history of BEM

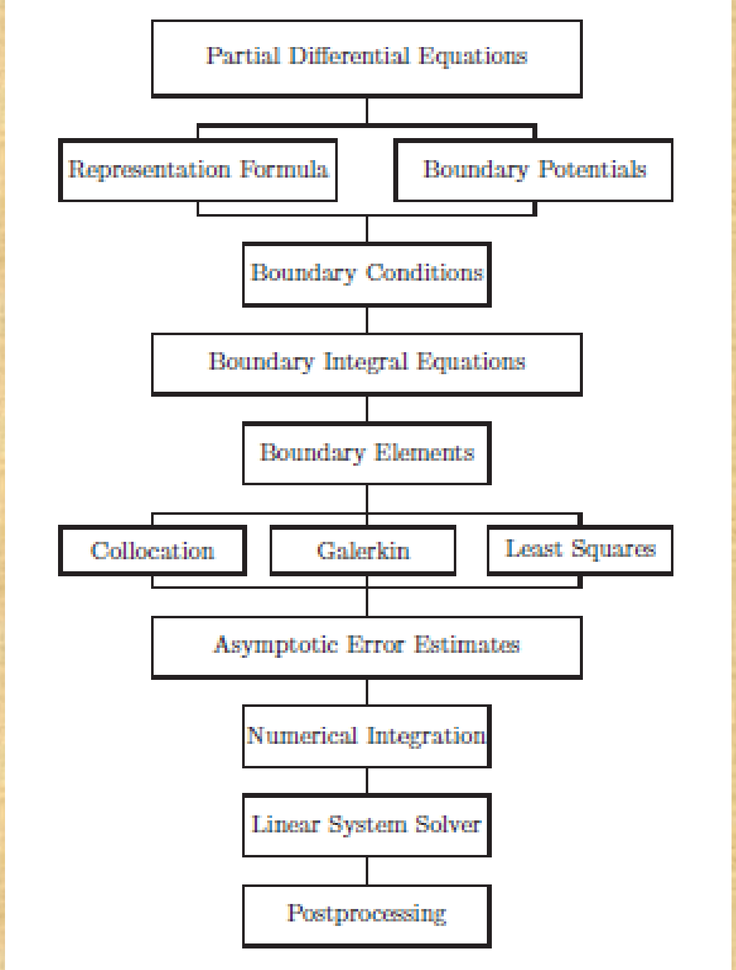
Precusrsors	Betti (1872), Somigliana (1885) working on elasticity and equilibrium; Fredholm (1903) established the theory of integral equations.
Origin	Jaswon (1963) and Symm (1963) can arguably be considered to have started BEM: They developed direct Boundary Integral Equation Methods (BIEM) for potential problems using Green's third identity.
Initial applications	Rizzo (1967) and Cruse (1969) developed BIE approaches for 2-D and 3-D elastostatic problems using Somigliana's identity and presented a formulation for transient elastodynamics employing the Laplace transform (Cruse & Rizzo (1968), Cruse (1968)).
BEM	Coined in 1977 in 3 publications: Banerjee & Butterfield (1977), Brebbia & Dominguez (1977), Dominguez (1977). The first book on the method appeared next year, written by Brebbia (1978).

Brief history of BEM

- Surge in research activities on the BEM since 1970's.
- The range of applications extended to other fields of mathematical physics such as electrodynamics and fluid mechanics.
- A common feature of all BEM is their use of fundamental solutions, which are free space solutions of the governing differential equations under the action of a point source.
  - The earliest fundamental solution for isotropic elastostatics stems from the 19th century and was derived by W. Thomson, later known as Lord Kelvin, in 1848.

A flowchart for BEM

- Central to the BEM is the reduction of boundary value problems to the equivalent integral equations on the boundary.
- It is well known that elliptic boundary value problems may have equivalent formulations in various forms of boundary integral equations. This provides a great variety of versions for BEMs.
- The terminology of BEM originated from the practice of discretizing the boundary manifold of the solution domain for the BIE into boundary elements, resembling the term of finite elements in FEM.
- In fact, the term BEM, nowadays denotes any efficient method for the approximate numerical solution of BIEs.



Boundary Element Methods – An Overview, G. C. Hsiao

Integral equations
General information

General form: $V(t) = \int_a^b K(x,t)\, \rho(t)\, dt$

where the functions $K(x,t)$, $V(t)$ and the limits a and b are known. The unknown $\rho(t)$ is to be obtained. The function $K(x,t)$ is called the kernel of the equation.

- First kind: Unknown found only within the integral sign
  - Fredholm equation: when limits a and b are fixed
  - Volterra equation: when one of the limits is variable
- Second kind: When the unknown is found also outside the integral sign written as follows (Fredholm equation)

$$\rho(t) = V(t) + \lambda \int_a^b K(x,t)\, \rho(t)\, dt$$

where λ can be an arbitrary complex parameter.

Boundary Integral Equation (BIE)

- An integral equation that is mathematically equivalent to the original partial differential equation and incorporates the boundary conditions.
- The essential re-formulation of the PDE consists of an integral equation that is defined on the boundary of the domain and an integral that relates the boundary solution to the solution at points in the domain.
- This is termed as the Boundary Integral Equation (BIE).
- An example from electrostatics will be presented next.

Electrostatics: Laplace's equation

$$\nabla^2\phi = \nabla\cdot(\nabla\phi) = 0$$

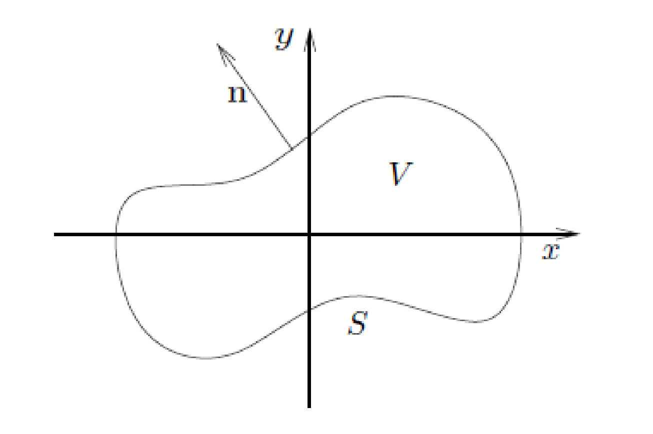
subject to boundary conditions of the type:

1. Dirichlet, where the unknown function is imposed on a portion of the boundary, i.e. $\varphi(x) = a(s)$, s being a coordinate system along the boundary.
2. Neumann, where the normal derivative of the function is known $\nabla\varphi \cdot n = q(s)$ where n is the outward unit normal.
3. Robin, where a relationship of the form $\alpha\varphi + \beta\nabla\varphi \cdot n = r(s)$.

A well-posed problem requires the specification of only one type of boundary conditions on any portion of the boundary, that is either the function value is specified, or the normal derivative but not both.

PDE -> BIE

- Poisson's equation in the open bounded region *V* with boundary *S*, $\nabla^2 u = F \text{ in } V.$ (1)



- According to the Green's theorem,

$$\int_V (u\nabla^2 v - v\nabla^2 u)\,\mathrm{d}V = \int_S \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}\right)\mathrm{d}S, \qquad (2)$$

where v is another function defined in V. Using (1), this leads to,

$$\int_V u\nabla^2 v\,\mathrm{d}V = \int_V vF\,\mathrm{d}V + \int_S \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}\right)\mathrm{d}S; \qquad (3)$$

Analytic Solutions of Partial Differential Equations (MATH 3414), School of Mathematics, University of Leeds

PDE -> BIE

- Now, if we choose $v \equiv v(x, \xi)$, singular at $x=\xi$, such that

$$\nabla^2 v = -\delta(\mathbf{x} - \boldsymbol{\xi})$$

- Then u is solution of the equation

$$u(\boldsymbol{\xi}) = -\int_V vF \, \mathrm{d}V - \int_S \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n} \right) \mathrm{d}S \qquad (4)$$

which is already an integral equation since u appears in the integrand.

PDE -> BIE

- Let us consider another function, $w \equiv w(x, \xi)$, regular at $x=\xi$, such that $\nabla^2 w = 0$ in V.
- Apply Green's theorem to the u and w:

$$\int_S \left(u\frac{\partial w}{\partial n} - w\frac{\partial u}{\partial n} \right) \mathrm{d}S = \int_V (u\nabla^2 w - w\nabla^2 u)\,\mathrm{d}V = -\int_V wF\,\mathrm{d}V. \qquad (5)$$

- Combining equations (4) and (5), we get

$$u(\xi) = -\int_V (v+w)F\,\mathrm{d}V - \int_S \left(u\frac{\partial}{\partial n}(v+w) - (v+w)\frac{\partial u}{\partial n} \right) \mathrm{d}S \qquad (6)$$

- If we consider the fundamental solution of Laplace's equation, $G = v+w$, such that $\nabla^2 G = -\delta(\mathrm{x} - \xi)$ in V,

$$u(\xi) = -\int_V GF\,\mathrm{d}V - \int_S \left(u\frac{\partial G}{\partial n} - G\frac{\partial u}{\partial n} \right) \mathrm{d}S.$$

- The way to remove u or $\partial u/\partial n$ from the RHS of the above equation depends on the choice of boundary conditions.

PDE -> BIE

- For example, let us consider the Dirichlet boundary condition, which implies $u = f$ on S. In order to eliminate $\partial u/\partial n$ from the RHS of (6), we may choose $w = -v$ on S, i.e. G=0 on S.
- Thus, the solution of the Dirichlet BVP for Poisson's equation $\nabla^2 u = F$ in V with $u = f$ on S is

$$u(\xi) = -\int_V GF\,\mathrm{d}V - \int_S f\frac{\partial G}{\partial n}\,\mathrm{d}S$$

- In this problem, $G = v+w$ (w regular at x=ξ) with $\nabla^2 v = -\delta(\mathrm{x}-\xi)$

and $\nabla^2 w = 0$ in V and $v+w = 0$ on S. So, G is the solution of the Dirichlet BVP $\nabla^2 G = -\delta(\mathrm{x}-\xi)$ in V, with G=0 on S.

Other Green's functions

- Those suitable for Neumann boundary conditions
- Those suitable for Robin boundary conditions
- Particularly important are the free space Green's functions. In particular, for Laplace equation in *n* dimensions:

$$v(\mathrm{x}, \xi) = \begin{cases} -\frac{1}{2}|x-\xi|, & n=1, \\ -\frac{1}{4\pi}\ln\left(|\mathrm{x}-\xi|^2\right), & n=2, \\ -\frac{1}{(2-n)A_n(1)}|\mathrm{x}-\xi|^{2-n}, & n\geq 3, \end{cases}$$

where x and ξ are distinct points and $A_n(1)$ denotes the area of the unit n-sphere.

Green's function

simple approach

$$\psi(\alpha) = \int G(\alpha, \beta) \cdot \rho(\beta)\, d\beta$$

- ψ represents the abstract state of an object – the effect. This state is dependent on α. α represents a variable like time or position, or both.
- $\rho(\beta)$ denotes the corresponding source / cause that depends on the variable β.
- The Green's function $G(\alpha, \beta)$ is the quantity that characterizes a certain object or a process with different objects involved (an interaction process, for example) and establishes a link between the state and the source.

Green's Functions in Classical Physics, Tom Rother, Springer, 2017

Green's function

Q&A

- We know the state of the object and the Green's function, and we ask for the source that is responsible for a certain state.
- We know the state and the source, and we ask for the Green's function that characterizes the object or the process this object gets involved in.
- We know the Green's function and the source, and we ask for the resulting state.
- Only the last question can be answered uniquely.

Detour: Green's function

historical point of view

George Green	**In 1828, published an *Essay on the Application of Mathematical Analysis to the Theory of Electricity and Magnetism:*** Green sought to determine the electric potential within a vacuum bounded by conductors with specified potentials. Famous Green's identities were proved for this purpose. (p1)
Arnold Sommerfeld	In the late 1890s, he developed a technique using integration on the complex plane to extend the method of images to several other useful geometries in three dimensions. Sommerfeld gave the free-space Green's function in two and three dimensions. More importantly, he derived his famous "radiation condition" that required outwardly propagating waves from physical considerations. (pp14-15)
P. M. Morse and H. Feshbach	The publication in 1946 of Methods of Theoretical Physics: "Green's function is the point source solution [to a boundary-value problem] satisfying appropriate boundary conditions." (p3)

Green's functions with Applications, Dean G.Duffy, Advances in Applied Mathematics, CRC Press, 2016

George Green: Detour ends

- Green's functions are named after George Green (1793–1841) of England.
- He was almost entirely self-taught in mathematics and made significant contributions to electricity and magnetism, fluid mechanics, and partial differential equations.
- His most important work was an essay on electricity and magnetism that was published privately in 1828. In this paper Green was the first to recognize the importance of potential functions.
- He introduced the functions now known as Green's functions as a means of solving boundary value problems and developed the integral transformation theorems, of which Green's theorem in the plane is a particular case.
- However, these results did not become widely known until Green's essay was republished in the 1850s through the efforts of William Thomson (Lord Kelvin).

Elementary Differential Equations and Boundary Value Problems, Boyce and DiPrima, John Wiley & Sons, 2009

BIE -> BEM

- The BEM is often referred to as *the boundary integral equation method* or *boundary integral method*. Since 1980-s, the term *boundary element method* has become more popular.
- The other terms are still used in the literature however, particularly when authors wish to refer to the overall derivation and analysis of the methods, rather than their implementation or application.
- An integral equation re-formulation can only be derived for certain classes of PDE. Hence the BEM is not widely applicable when compared to the near-universal adaptability of the finite element and finite difference method.

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

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

Potential at r

Charge density at r'

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

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

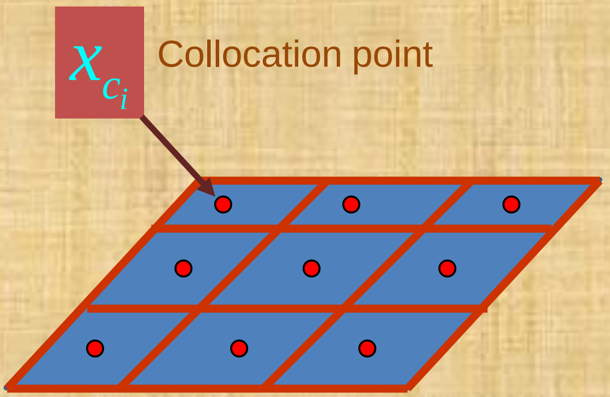
Accuracy depends critically on the estimation of [A], in turn, the integration of G, which involves singularities when r → r'.

Most BEM solvers fail here.

Conventional BEM

Centroid Collocation

Basis Function Approach



Singularity is located and boundary condition is satisfied at the nodal points

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

Single point quadrature $A_{i,j} \approx \dfrac{Panel\ \ Area}{\left\| x_{c_i} - x_{centroid_j} \right\|}$

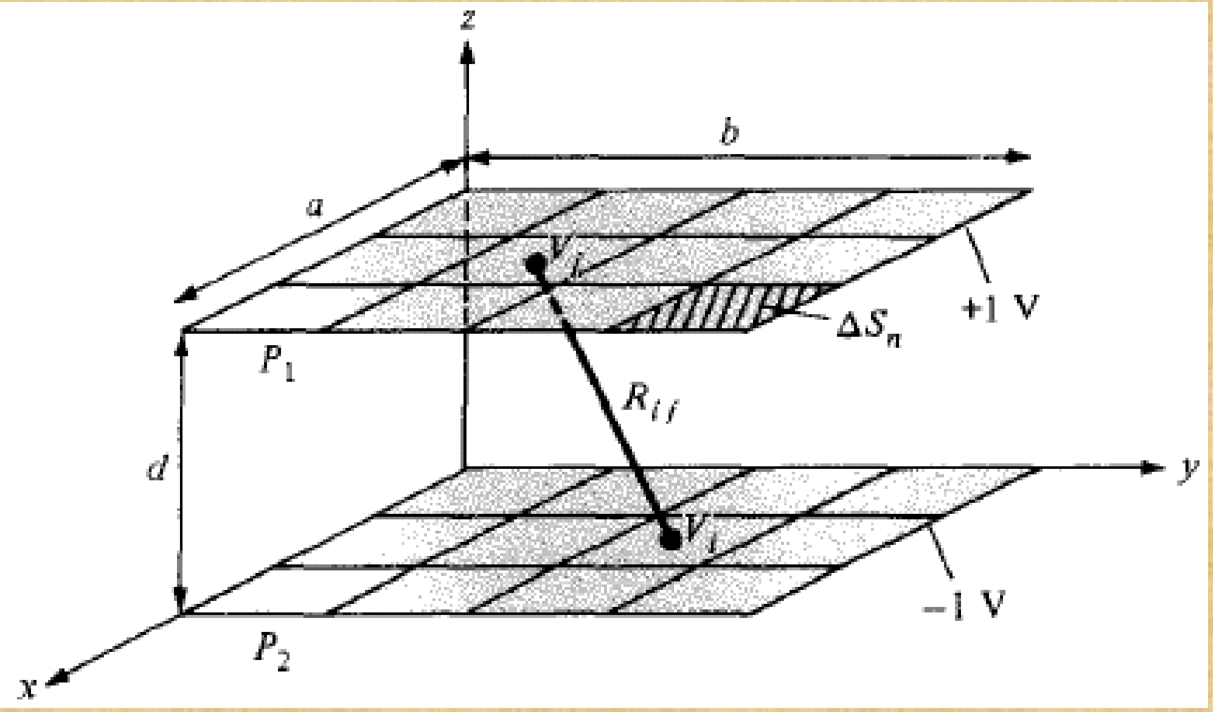
$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \vdots \\ \alpha_n \end{bmatrix} = \begin{bmatrix} \Psi\left(x_{c_1}\right) \\ \vdots \\ \vdots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

- Deals with nodal singularities and, thus, near-field estimates are erroneous and lead to numerical boundary layer: geometric singularity and physical singularity
- Special treatment is necessary for self-influence.

Conventional BEM

The capacitance problem

Typical text-book problem: Use the method of moments / boundary element method to find the capacitance of the parallel plate capacitor shown below. Take a = 1m, b = 1m, d = 1m and $\varepsilon_r = 1.0$. Let the top plate be at +1V and the bottom plate at -1V.



Capacitance problem

Steps

1) Discretize the plate P_1 into *1 … n* elements and P_2 into *(n+1) … 2n* elements,
2) Assuming uniform charge density (piecewise constant basis function) on each element, find surface charge density on each of the elements on the plates P_1 and P_2,
3) Get total charge, Q, on each plate by integrating the surface charge density on the plate,
4) C = Q / V = Q / 2.0

Capacitance problem

Steps

Potential V_i at the collocation point of an element *i* is

$$V_i = \int_S \frac{\rho_S \, dS}{4\pi\varepsilon_o R} \simeq \sum_{j=1}^{2n} \frac{1}{4\pi\varepsilon_o} \int_{\Delta S_i} \frac{\rho_j \, dS}{R_{ij}}$$
$$= \sum_{j=1}^{2n} \rho_j \frac{1}{4\pi\varepsilon_o} \int_{\Delta S_i} \frac{dS}{R_{ij}}$$

If we define A_{ij} as

$$A_{ij} = \frac{1}{4\pi\varepsilon_o} \int_{\Delta S_i} \frac{dS}{R_{ij}}$$

V_i become

$$V_i = \sum_{j=1}^{2n} \rho_j A_{ij}$$

Capacitance problem

Influence coefficient matrix

Arranging the expressions for all the elements (i = 1, …, n, (n+1), …, 2n), we get

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1,2n} \\ A_{21} & A_{22} & \cdots & A_{2,2n} \\ \vdots & & & \vdots \\ A_{2n,1} & A_{2n,2} & \cdots & A_{2n,2n} \end{bmatrix} \begin{bmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_{2n} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ -1 \\ -1 \end{bmatrix}$$

If we consider the elements to be square of side Δl,

$$A_{ij} = \frac{\Delta S_i}{4\pi\varepsilon_o R_{ij}} = \frac{(\Delta\ell)^2}{4\pi\varepsilon_o R_{ij}} \qquad i \neq j$$

$$A_{ii} = \frac{\Delta\ell}{\pi\varepsilon_o} \ln(1 + \sqrt{2}) = \frac{\Delta\ell}{\pi\varepsilon_o} (0.8814)$$

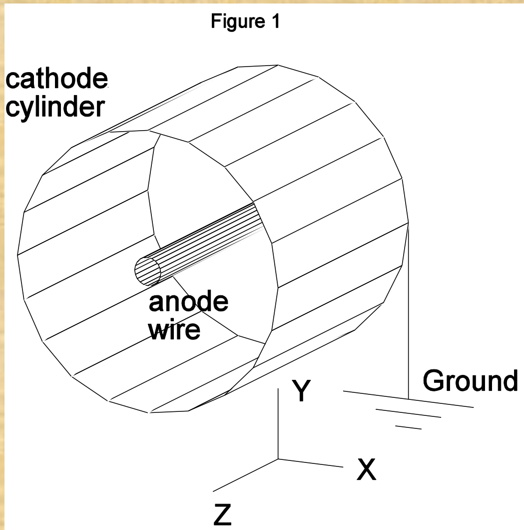
Capacitance problem

Final steps

- So, all we need to know now is the influence coefficient or capacitance matrix, which depends, in this case, entirely on the geometry of the problem
- Iterate or invert the matrix to get the charge density on each element
- Sum the charge on a plate
- Estimate the capacitance
- Find potential and field at any given point, if we want (how?)
- What happened to the far-field boundary condition?

A cylindrical proportional counter

Comparison of analytical and computed potential fields



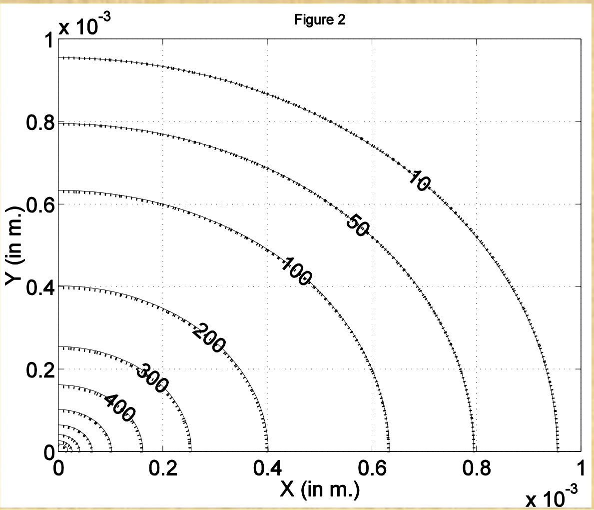
Geometry of a cylindrical proportional counter

Collocation BEM

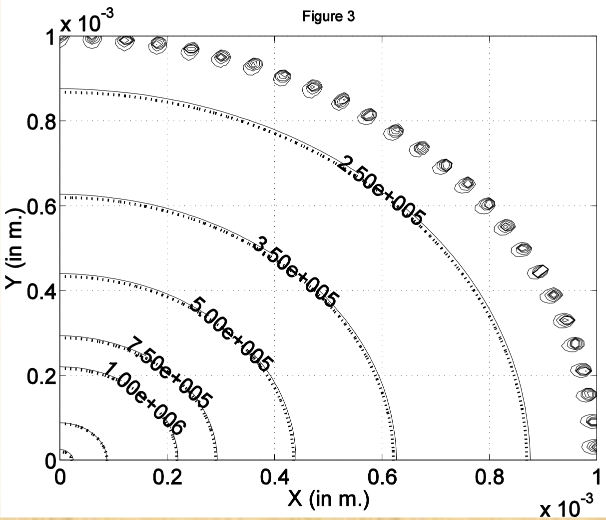
Not good enough even for a very simple geometry!

Edge effects studied, thanks to numerical implementation

Acceptable potential



Acceptable field (?)



Conventional BEM

not good enough

Major Approximations

- 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.

Numerical boundary layer

Constant element approach

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

BEM Basics
Singularities

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

Comparison among BEM Variants

	Advantages	Disadvantages
CBEM	• Easiest to implement • Fast solution • Applicable to wide range of standard cases	• Poor convergence and accuracy • Nonsymmetrical and dense matrices • Difficult to deal with hypersingular integral
GBEM	• High accuracy • Able to handle singular and hypersingular integrals • Easier to produce symmetric coefficient matrix • Can be implemented for various problems including	• Slow solution
DRBEM	• Able to deal with domain integrals • Requires only boundary discretization • Applicable to wide range of problems	• Fully populated and nonsymmetrical matrices • Computationally expensive • Mathematically complicated
CVBEM	• High accuracy • Suitable for problems with stress singularities and concentrations	• Limited to Laplace-type problem
AEM	• Able to deal with domain integrals • Requires only boundary discretization • Suitable for linear and nonlinear problem	• Mathematically complicated • Limited applicability • Hard to implement

Yu et al., EABE 34 (2010) 884–899

Major

Issues

- Ease of implementation
- Speed of execution
- Range of problems accessible
- Precision
- Ability to handle singularities
- Nature of coefficient matrix
- Surface / Domain integration
- Complexity of mathematics

nearly exact BEM (neBEM)

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.

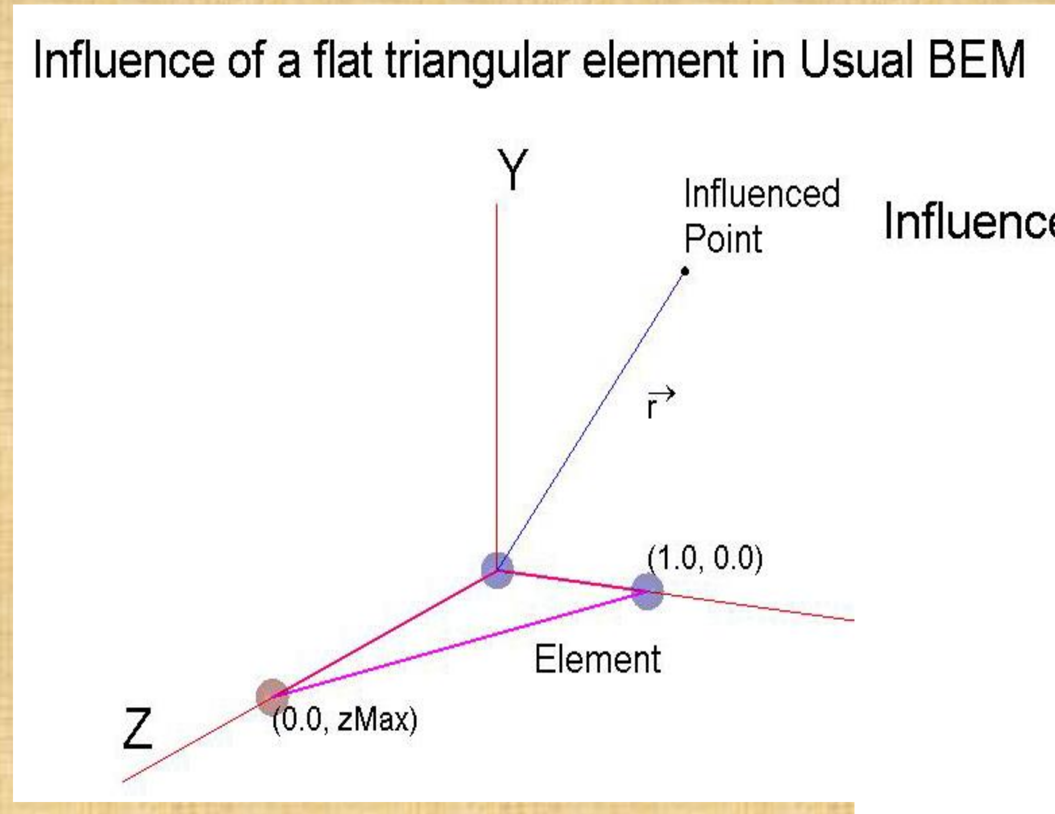
Restatement of the approximations

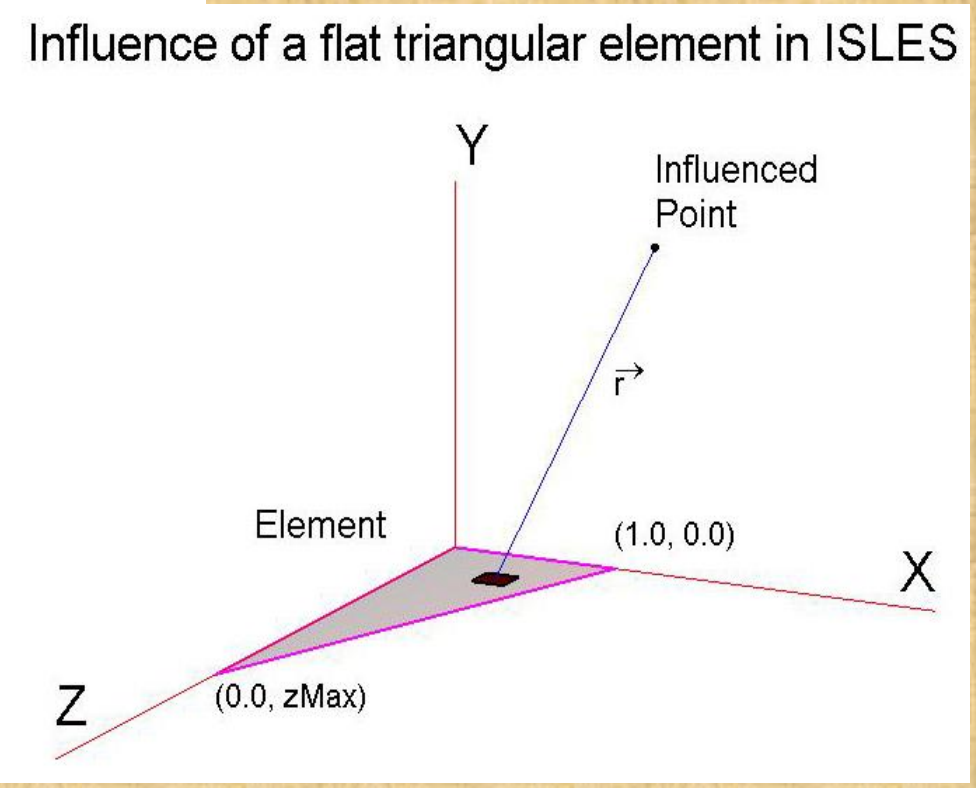
- Singularities distributed uniformly on the surface of boundary elements
- Strength of the singularity changes from element to element.
- Strengths of the singularities solved depending upon the boundary conditions, modeled by the shape functions

ISLES library and neBEM Solver

Foundation expressions are analytic and valid for the complete physical domain

Contrast of approaches
nodal versus distributed

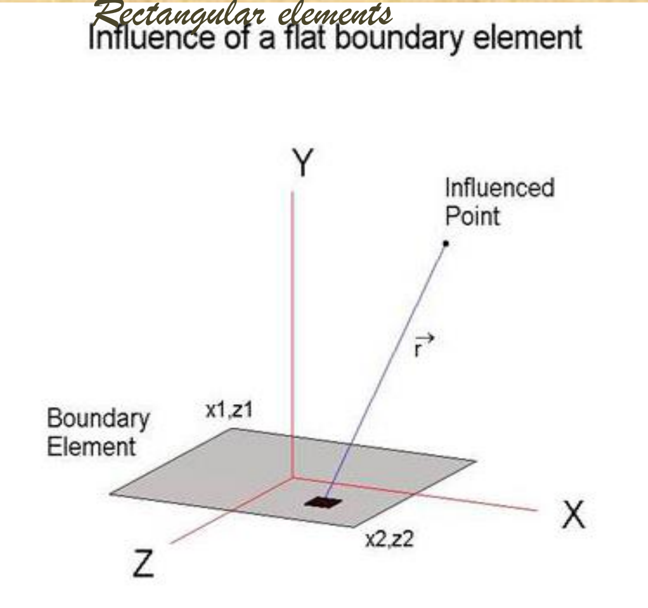




Inverse Square Law Exact Solutions (ISLES)

Foundation expressions of ISLES

Rectangular elements



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

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

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

4 log terms

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

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

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

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

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

May need translation and vector rotation

$$F_X(X,Y,Z) = \ln\left(\frac{D_{i,j} - (Z - z_j)}{D_{m,n} - (Z - z_n)}\right) \Rightarrow \text{2 terms}$$

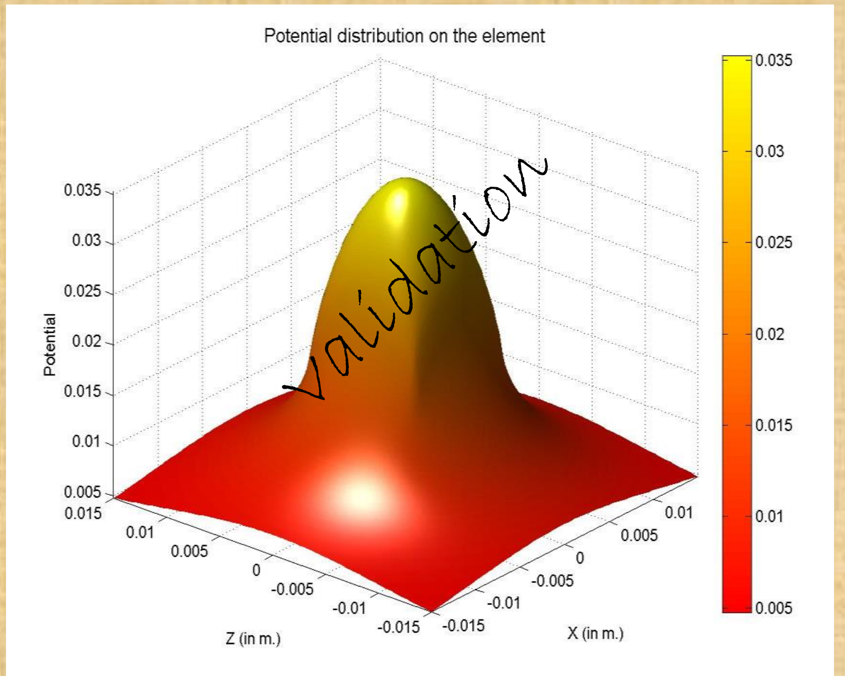
$$F_Y(X,Y,Z) =$$

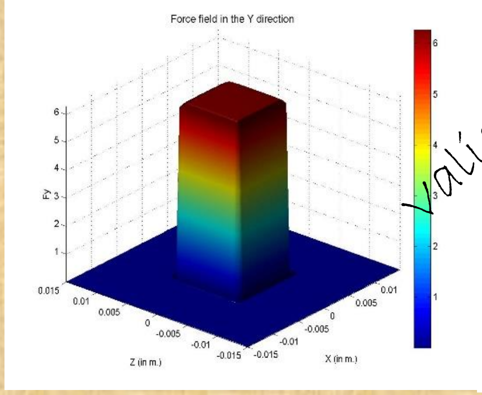
$$-\frac{i}{2}\,Sign(Y) \times \left\{ \begin{aligned} & S_j \tanh^{-1}\left(\frac{R_j + iI_i}{D_{i,j}\left|Z - z_j\right|}\right) \\ & + S_j \tanh^{-1}\left(\frac{R_j - iI_i}{D_{i,j}\left|Z - z_j\right|}\right) \end{aligned} \right\} + C \Rightarrow \text{4+4 terms}$$

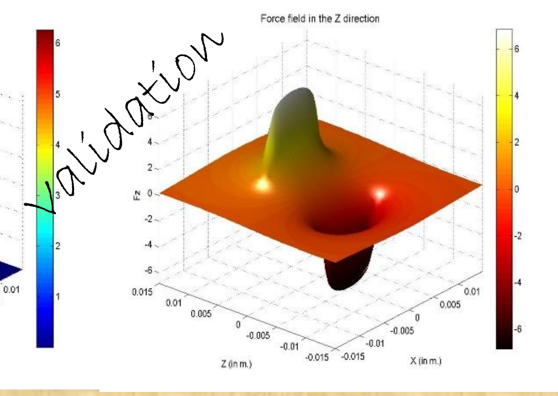
$$F_Z(X,Y,Z) = \ln\left(\frac{D_{i,j} - (X - x_i)}{D_{m,n} - (X - x_m)}\right) \Rightarrow \text{2 terms}$$

C is a constant of integration as follows :

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

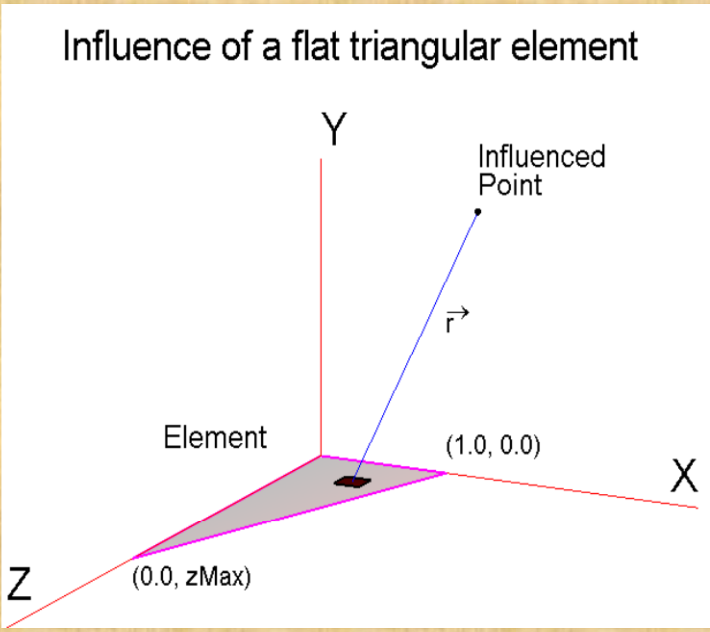






Foundation expressions of ISLES

Triangular element



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

Please note the integration limits: while any length is allowed in one co-ordinate, the other can be varied from 0 to 1, only.

$$\begin{aligned}\Phi = \frac{1}{2}\Bigg(& (z_M Y^2 - XG)(LP_1 + LM_1 - LP_2 - LM_2) \\ & + \mathrm{i}|Y|(z_M X + G)(LP_1 - LM_1 - LP_2 + LM_2) \\ & - S_1 X\left(\tanh^{-1}\left(\frac{R_1 + \mathrm{i}I_1}{D_{11}|Z|}\right) + \tanh^{-1}\left(\frac{R_1 - \mathrm{i}I_1}{D_{11}|Z|}\right)\right. \\ & \left. -\tanh^{-1}\left(\frac{R_1 + \mathrm{i}I_2}{D_{21}|Z|}\right) - \tanh^{-1}\left(\frac{R_1 - \mathrm{i}I_2}{D_{21}|Z|}\right)\right) \\ & + \mathrm{i}S_1|Y|\left(\tanh^{-1}\left(\frac{R_1 + \mathrm{i}I_1}{D_{11}|Z|}\right) - \tanh^{-1}\left(\frac{R_1 - \mathrm{i}I_1}{D_{11}|Z|}\right)\right. \\ & \left. -\tanh^{-1}\left(\frac{R_1 + \mathrm{i}I_2}{D_{21}|Z|}\right) + \tanh^{-1}\left(\frac{R_1 - \mathrm{i}I_2}{D_{21}|Z|}\right)\right) \\ & + \frac{2G}{\sqrt{1+z_M^2}}\log\left(\frac{\sqrt{1+z_M^2}D_{12} - E_1}{\sqrt{1+z_M^2}D_{21} - E_2}\right) \\ & + 2Z\log\left(\frac{D_{21} - X + 1}{D_{11} - X}\right)\Bigg) + C\end{aligned}$$

Similar expressions as for rectangular elements but much longer with larger number of definitions and constants of integration.

May need translation, vector rotation and simple scalar scaling

Foundation expressions of ISLES

Straight thin wire element

$$\phi(X,Y,Z) = 2\pi a \log\left(\frac{\sqrt{X^2+Y^2+(h+Z)^2}+(h+Z)}{\sqrt{X^2+Y^2+(h-Z)^2}-(h-Z)}\right)$$

$$F_x(X,Y,Z) = 2\pi a X\left(\frac{(h-Z)\sqrt{X^2+Y^2+(h+Z)^2}+(h+Z)\sqrt{X^2+Y^2+(h-Z)^2}}{(X^2+Y^2)\sqrt{X^2+Y^2+(h-Z)^2}\sqrt{X^2+Y^2+(h+Z)^2}}\right)$$

$$F_y(X,Y,Z) = 2\pi a Y\left(\frac{(h-Z)\sqrt{X^2+Y^2+(h+Z)^2}+(h+Z)\sqrt{X^2+Y^2+(h-Z)^2}}{(X^2+Y^2)\sqrt{X^2+Y^2+(h-Z)^2}\sqrt{X^2+Y^2+(h+Z)^2}}\right)$$

$$F_z(X,Y,Z) = 2\pi a\left(\frac{\sqrt{X^2+Y^2+(h+Z)^2}-\sqrt{X^2+Y^2+(h-Z)^2}}{\sqrt{X^2+Y^2+(h+Z)^2}\sqrt{X^2+Y^2+(h-Z)^2}}\right)$$

Ring made of thin wire element

- Potential and flux are obtained from expressions involving combination of elliptic functions and relatively benign algebraic expression involving the usual trigonometric functions
- Implementation of these expressions into ISLES is complete.

Charged disc: Difficult work under way.

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

Validation: Classical Problems

Capacitance of a unit square plate and a square cube

- Capacitance of an isolated plate and an isolated cube - two major unsolved problems of electrostatics.
- No analytic values exist.
- Numerous attempts:
  - Begins with Maxwell's computations
  - BEM, Surface Charge Method, Extrapolation
  - Random-walk on boundary, Refinements
  - Walk on Spheres, Refinements
  - Brownian dynamics, Refinements
- Please note
  - Following values are normalized by $4\pi\varepsilon_0 l$ where l is length of a side.
  - The error ranges have been omitted to accommodate a large number of values in the Table.

Classical Problems

Numerous attempts …

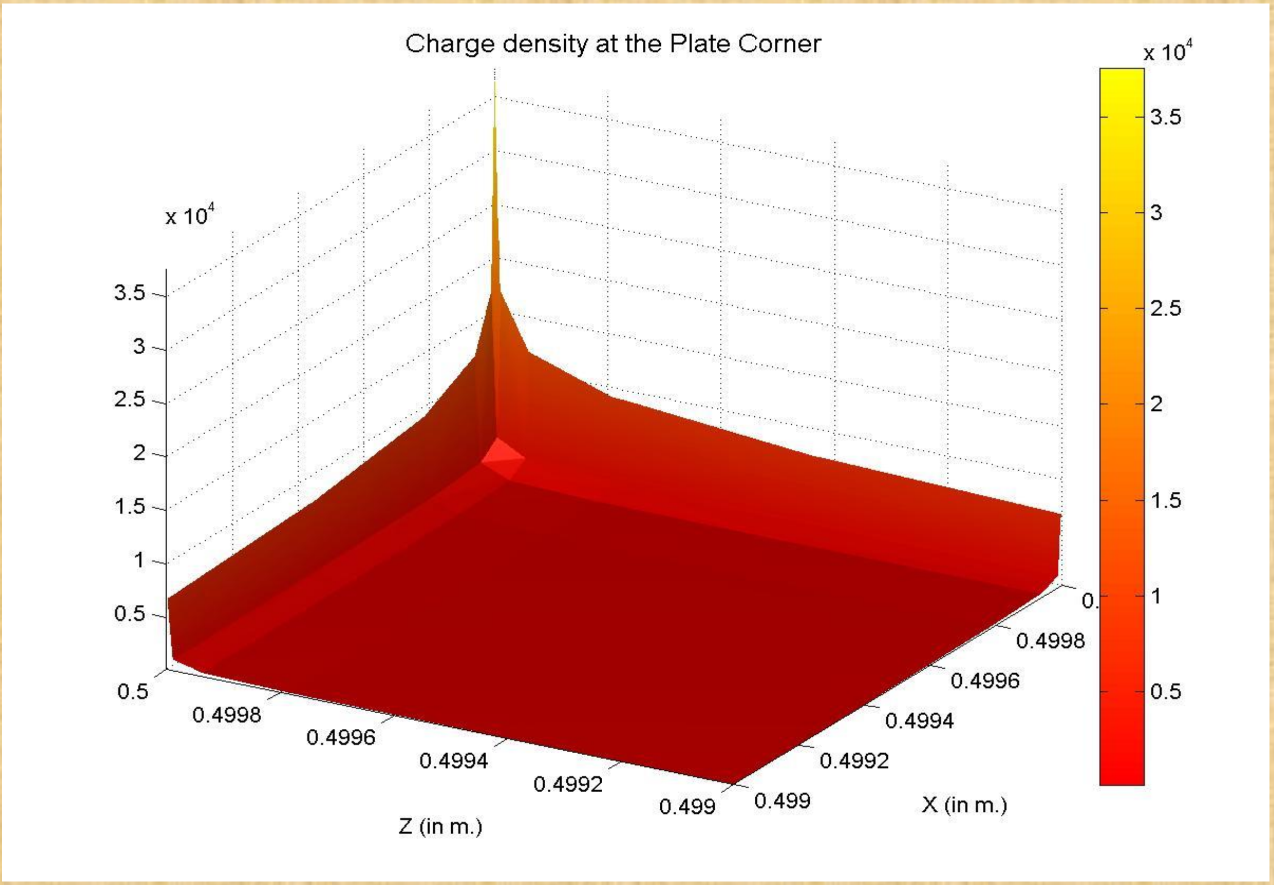
- In a recent work (based on random walk):
  - Lower bound for cube: 0.6596
  - Capacitance for cube: 0.6606 ± 0.0001
  - Capacitance for plate: 0.36 ± 0.01
  - Upper bound for cube: 0.6619
- BEM has been criticized
  - For its inability to handle corner singularities.
  - As outer contour points reach the edge, the results found to vary markedly as a function of the number of meshes.
  - Oscillation in the charge density near corners / edges (especially for plates).

Electrostatic problems - capacitance

Classical problems of electrostatics: (a) a conducting plate raised to one volt, (b) a conducting cube raised to one volt

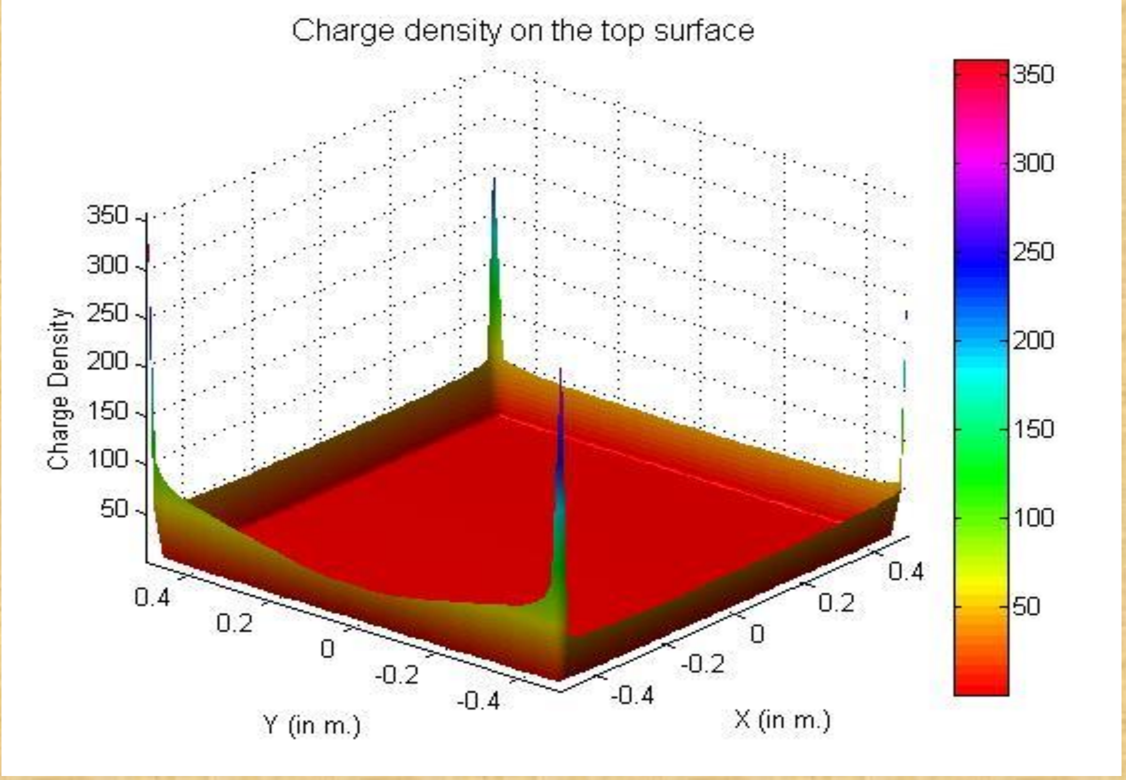
Reference	Method	Plate	Cube
Maxwell	SCM	0.3607	-
Reitan, Higgins	SCM	0.362	0.6555
Solomon	SCM	0.367	-
Goto, Shi, Yoshida	Refined SCM, Extrapolation	0.3667892	0.6606747
Douglas, Zhou, Hubbard	Brownian Dynamics (BD)	-	0.663
Read	Refined BEM, Extrapolation	0.3667874	0.6606785
Given, Hubbard, Douglas	RBD	-	0.660675
Mansfield, Douglas, Garboczi	Numerical Path Integration	0.36684	0.66069
Hwang, Mascagni	Walk on Spheres (WOS)	-	0.660683
Hwang	Modified WOS	-	0.6606867
Mascagni, Simonov	Random Walk on the Boundary	-	0.6606780
Wintle	Random walk	0.36	0.6606
Present	Nearly Exact BEM	0.3667869	0.6606746

No dips



Charge density at the Plate Corner
x 10^4
3.5
3
2.5
2
1.5
1
0.5
0.5
0.4998
0.4996
0.4994
0.4992
0.499
Z (in m.)
0.499
0.4992
0.4994
0.4996
0.4998
X (in m.)

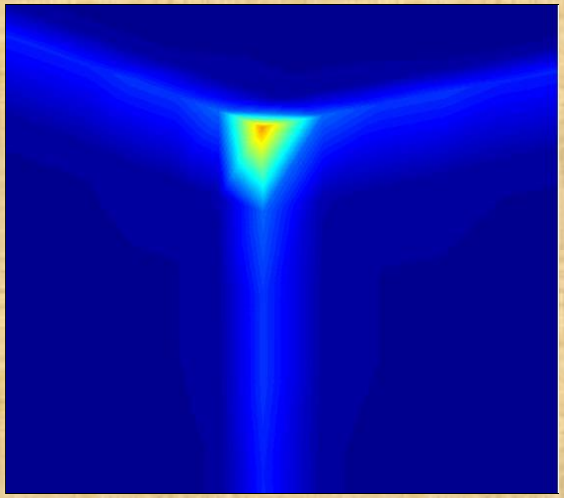
Smooth variations



Length scales

A micron in a meter – extremely difficult for FEM

One of the major unsolved problems of electrostatics – a unit conducting cube raised to unit volt – an excellent benchmark

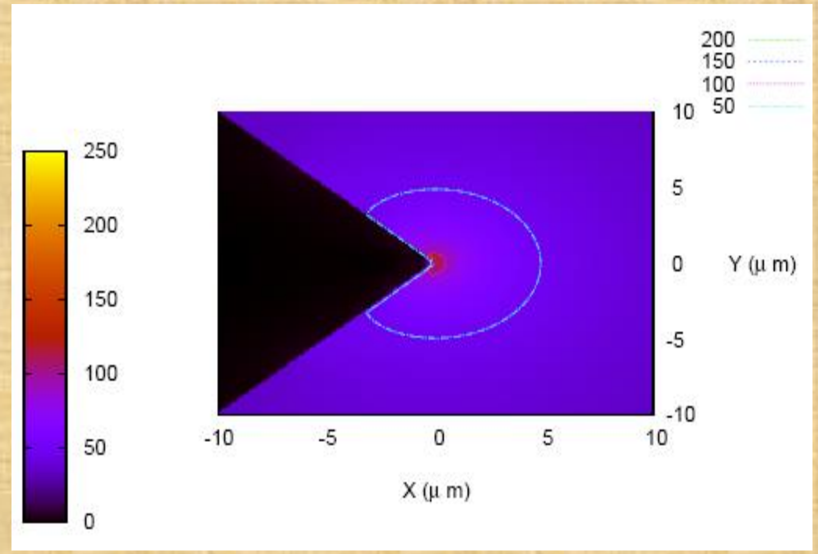


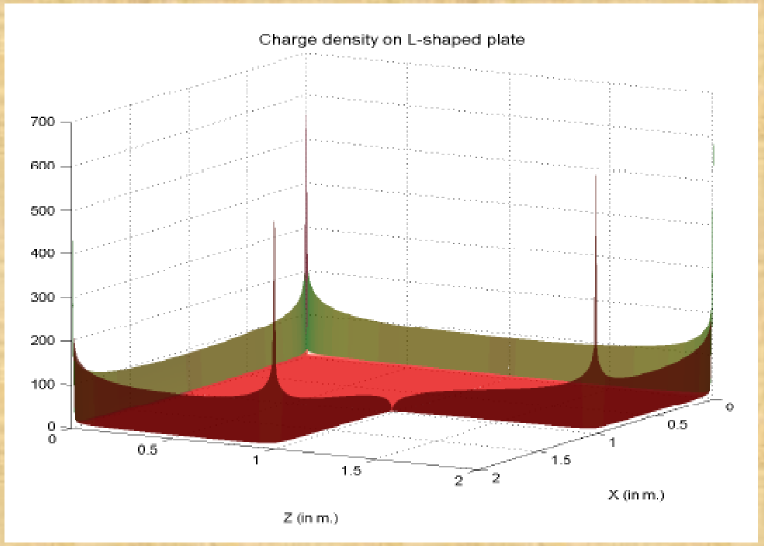
Charge density distribution at one of the corners

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

Intricate geometries

sharp corners

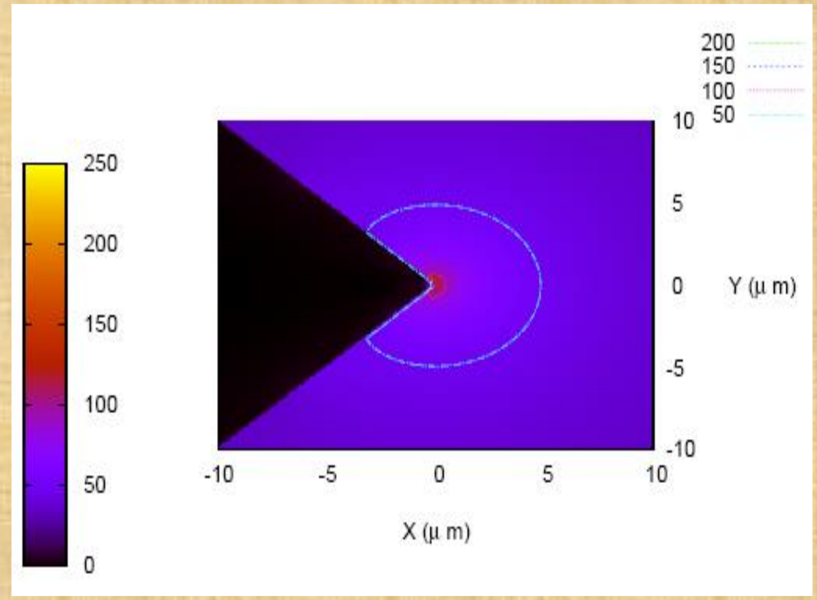




- Electrostatics of both inner and outer corners have been estimated
- It has been possible to estimate field to within 5% for a point within a micron of a convex corner
- For a concave corner, usable estimation could be made upto within 10 microns of 90^{o} corner

Intricate geometries

Sharp corners – extremely difficult for FEM



Electric field close to a 270° edge

Distance	Analytical	ELECTRO	Error (%)	neBEM	Error (%)
0.8	0.5246997	0.524710	0.0019	0.5241510	−0.105
0.1	1.747623	1.747621	0.00014	1.747953	−0.018
0.01	3.931433	3.931284	0.0038	3.933242	−0.046
0.001	8.487415	8.4854	0.023	8.491335	−0.046
0.0001	18.28732	18.202	0.46	18.29270	−0.029
0.00001	39.39902	35.80	9.1	39.30955	−0.227
0.000001	84.88264	57.10	32.7	80.74309	−4.877

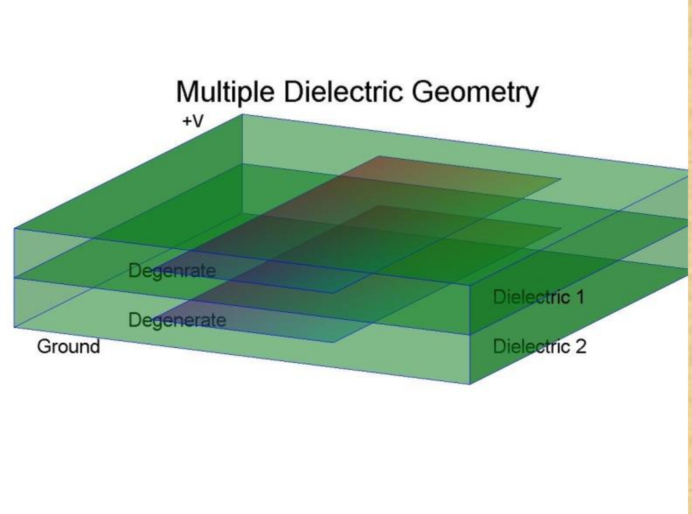
Electric field close to a 360° edge

Distance	Analytical	ELECTRO	Error (%)	neBEM	Error (%)
0.8	0.3954180	0.3954213	0.00059	0.3950786	−0.086
0.1	1.830153	1.830155	0.00010	1.830110	−0.002
0.01	6.303166	6.303172	0.000094	6.305784	−0.041
0.001	20.11157	20.11122	0.0018	20.11963	−0.04
0.0001	63.65561	63.64274	0.020	63.64780	−0.012
0.00001	201.3148	200.88	0.22	200.5488	−0.3
0.000001	636.6191	621.25	2.4	621.6034	−2.36

- 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 (shown in the next slide)

Multiple dielectric systems

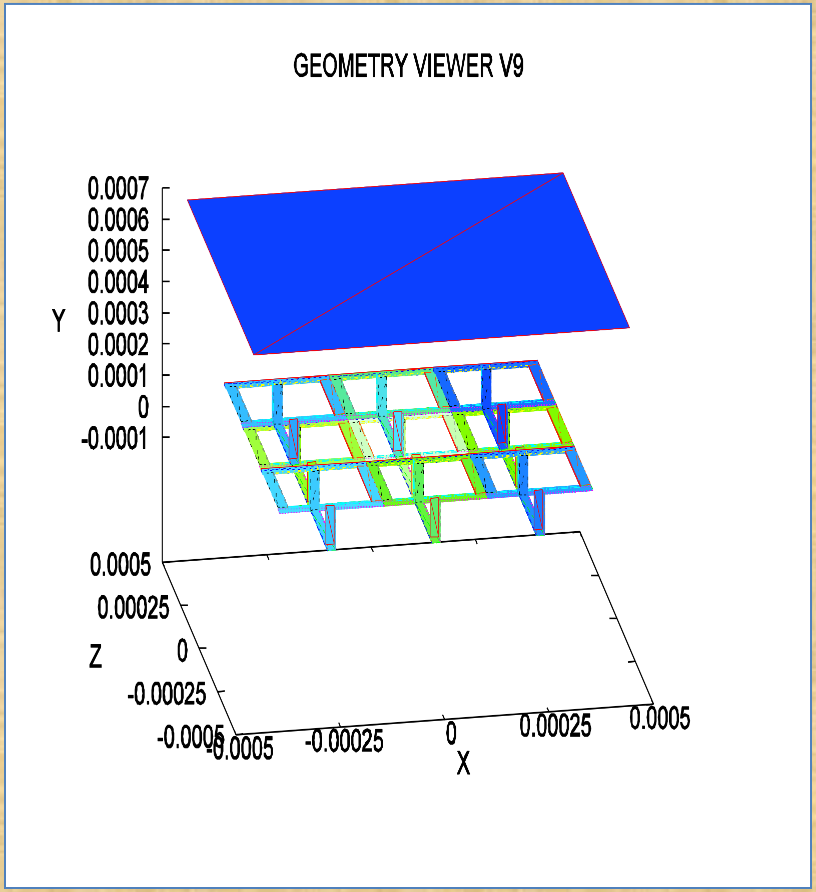
Two dimensional model problem with degenerate conducting surfaces solved using the Dual BEM (DBEM) and compared with FEM in Chyuan et. al. [(Semicond. Sci. Technol. 19 (2004)]

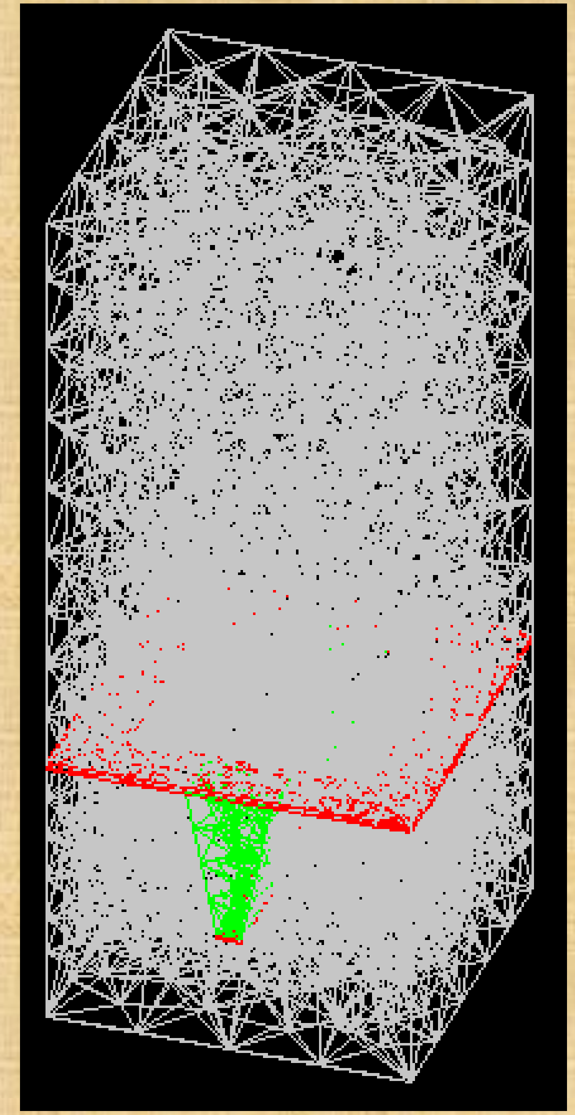


Degenerate	Ratio of dielectrics = 10		
Location	FEM	DBEM	Present
24.0,16.5	0.514489	0.52181	0.5247903
6.5,12.0	0.2301575	0.23801	0.2398346
22.5,6.0	0.3638855	0.34638	0.3451232
4.0,3.5	0.1108643	0.10623	0.1058357

Non-degenerate	Ratio of dielectrics = 10			Ratio of dielectrics = 0.1		
Location	FEM	DBEM	Present	FEM	DBEM	Present
18.0,3.0	0.1723103	0.17302	0.1740844	0.01741943	0.017302	0.01771752
4.0, 9.0	0.2809692	0.27448	0.2807477	0.0281006	0.027448	0.0286358
25.0, 16.0	0.6000305	0.59607	0.5991884	0.48833313	0.480640	0.4828946
5.0,17.0	0.679071	0.67492	0.6785017	0.5929200	0.589690	0.5926387

Micro-wire detector

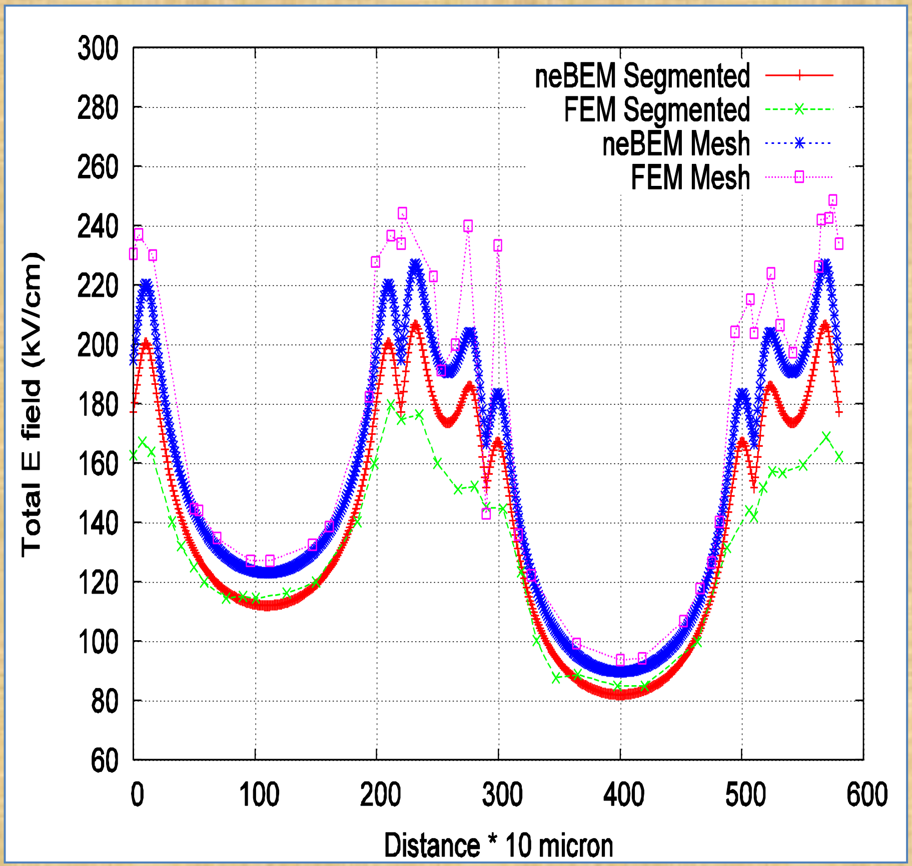




Surface elements vs Volume elements

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!
- 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 fluctuates and is the results near and at the edges are doubtful

nearly exact Boundary Element Method (neBEM)

A new formulation based on green's function that allows the use of exact close-form analytic expressions while solving 3d problems governed by Poisson's equation. It is very precise even in critical near-field regions, and microscopic length scale.

It is easy to use, interface and integrate neBEM

Stand-alone
A driver routine
An interface routine
Post-processing

Garfield
Garfield prompt
Garfield script

Charge density at all the interfaces

Potential at any arbitrary point

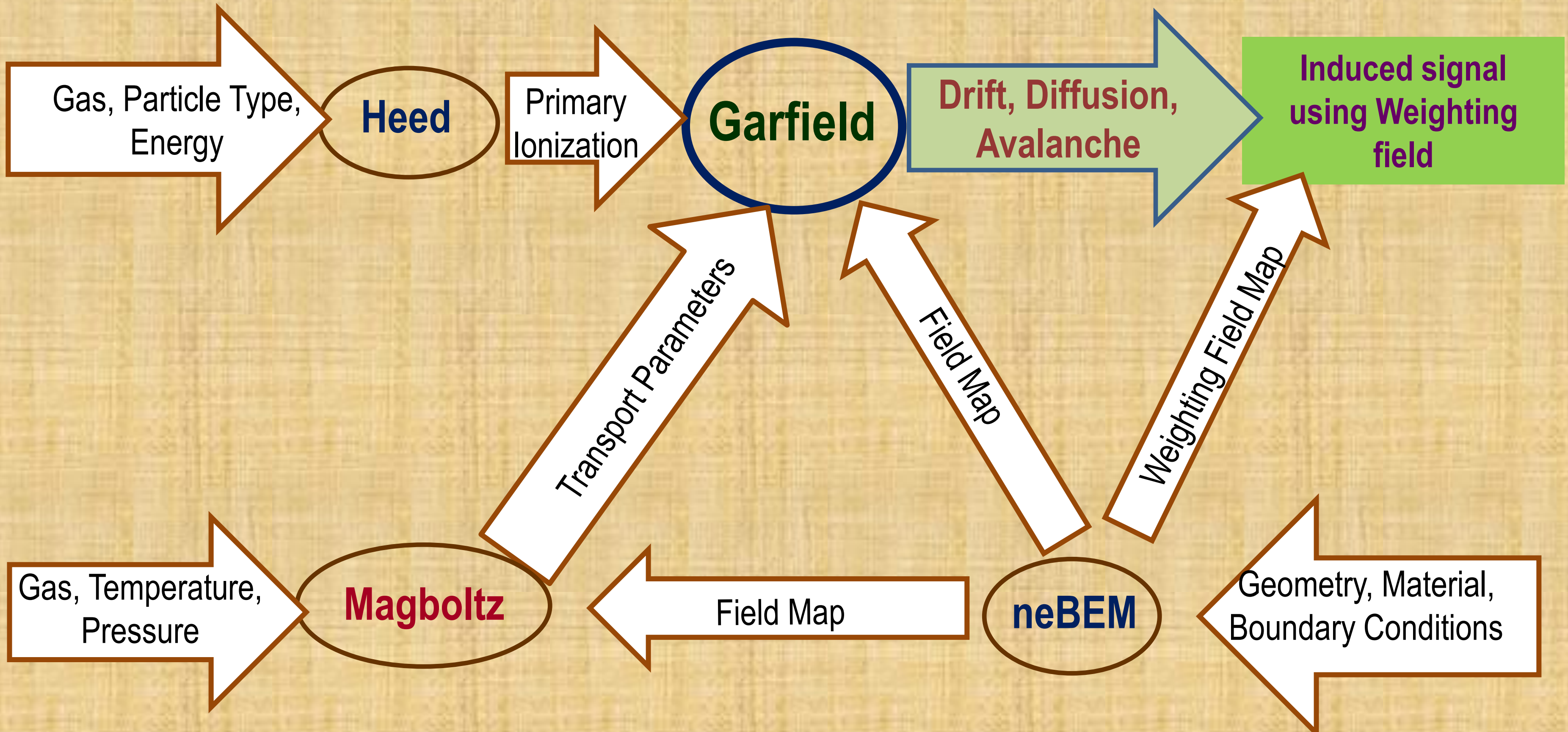
Field at any arbitrary point

Capacitance, forces on device components properties can be obtained by post-processing

neBEM@CERN

http://nebem.web.cern.ch

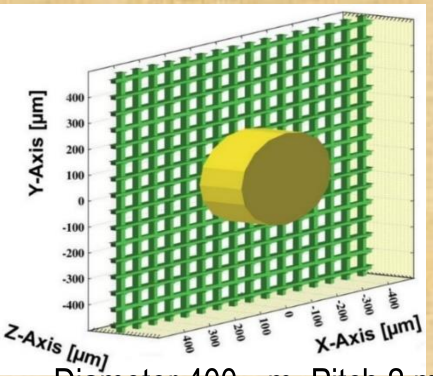
RD51 simulation framework



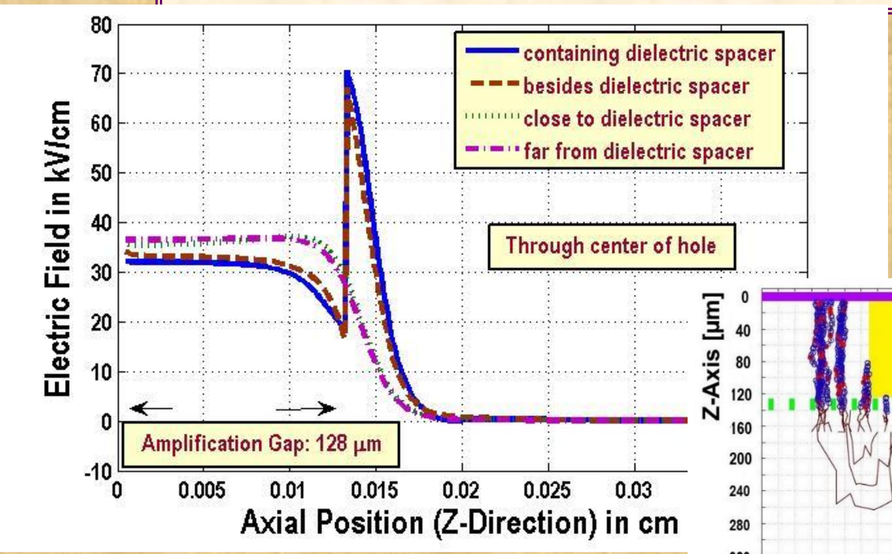
neBEM interface to Garfield++: To be discussed by Heinrich Schindler in WG4, 10:40 CET, 25 June 2020

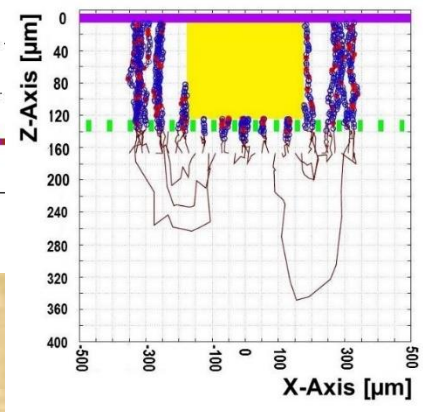
Position resolution: Effect of Spacers

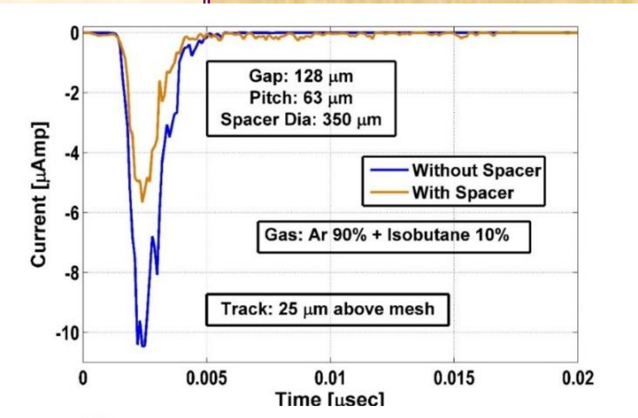
- ✓ Spacers cause significant perturbation resulting in increased field values, particularly in the regions where cylinders touch the mesh
- ✓ Electron drift lines get distorted near the spacer, some electrons are lost on it, resulting in a reduced gain
- ✓ Due to the reduced gain, electron signal strength gets affected significantly, the signal profile consists of a long tail resulting from the distorted drift
- ✓ Due to the dead regions introduced by the spacer, the readout pads below or close to the spacers are found to be affected which leads to inefficiencies in track reconstruction

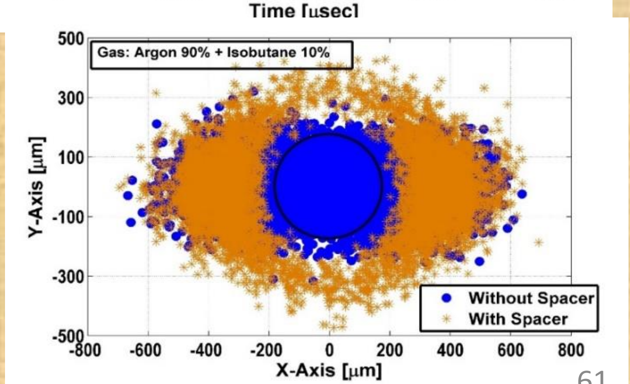


Diameter 400 μm, Pitch 2 mm

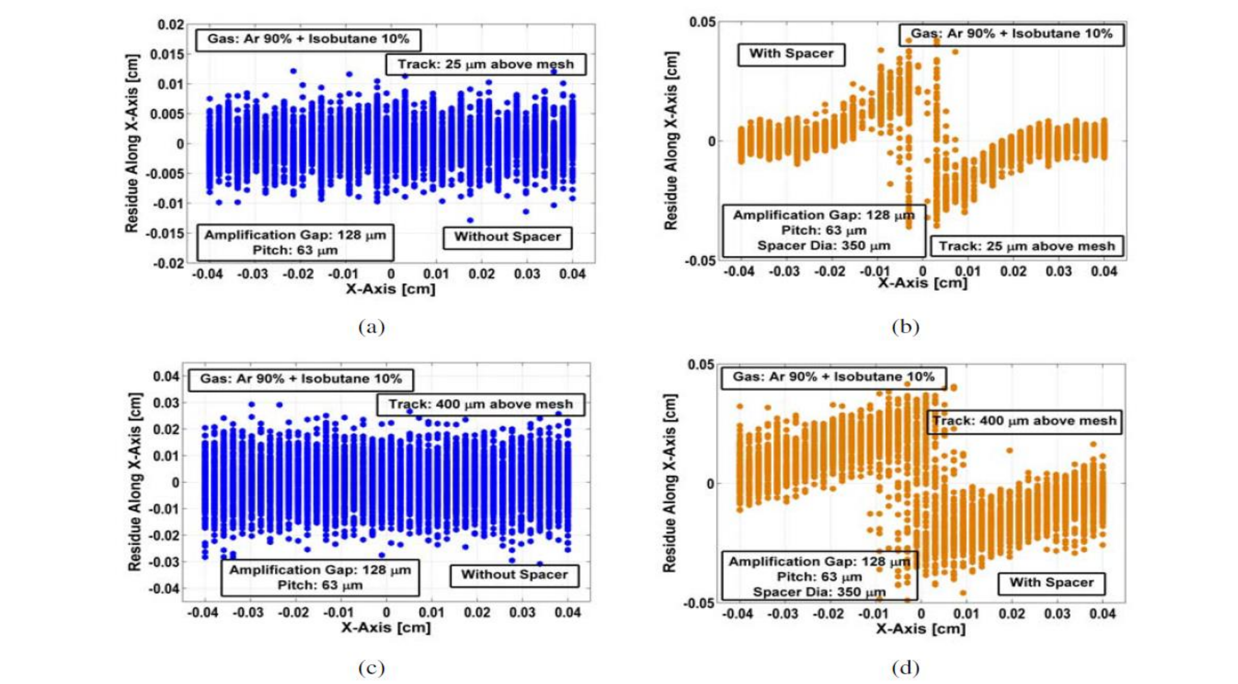




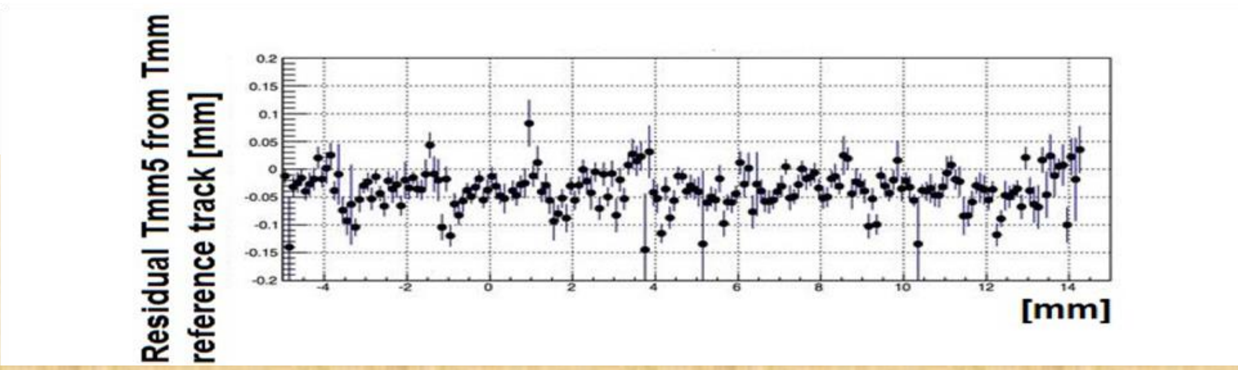




Effect of spacer on position resolution

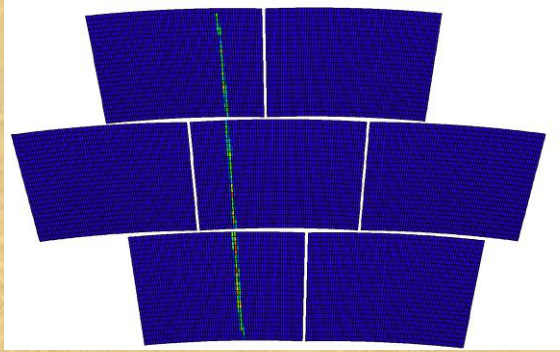


The simulated residue without a spacer from a track (a) 25 μm and (c) 400 μm above the micromesh; with a spacer from a track (b) 25 μm and (d) 400 μm above the micromesh, for the bulk Micromegas having amplification gap of 128 μm and pitch of 63 μm. Spacer diameter = 350 μm, drift field = 200 V/cm.

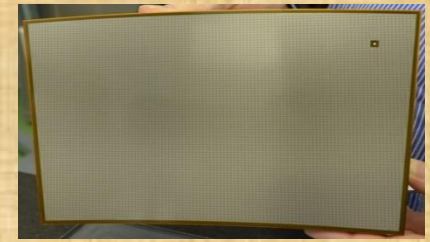


The experimental residual plot in Ar-CO2 mixture, observed in the test beam run of August 2014 by the ATLAS group working for the MAMMA project

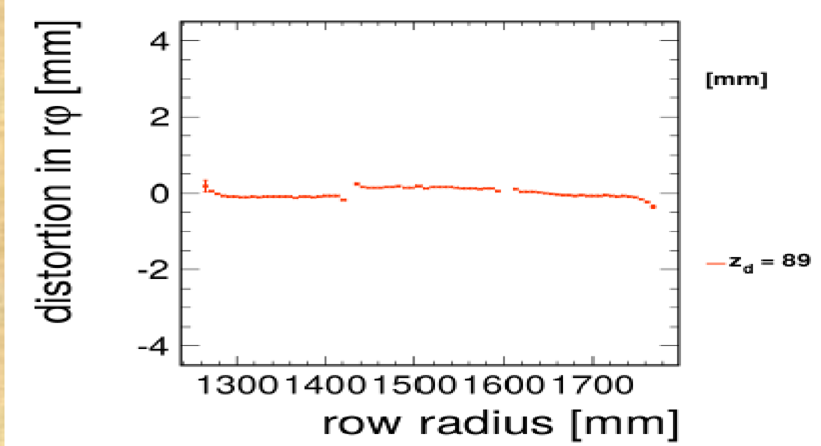
Distortion in Micromegas based TPC @ ILC



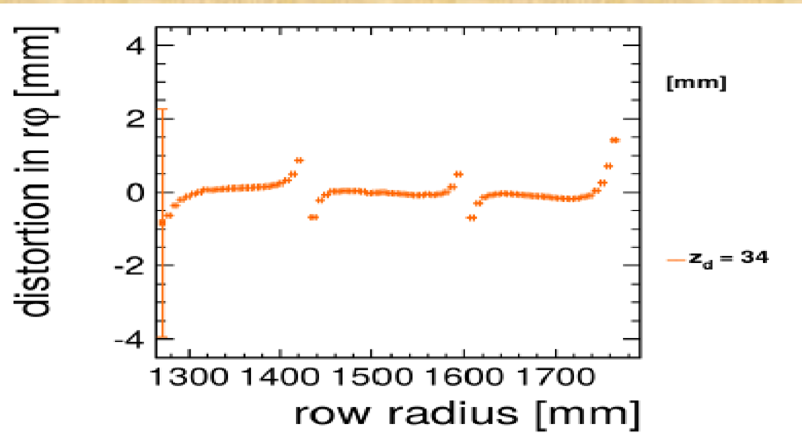
All modules are identical keystone shaped.
Gap between the modules = 3 mm



A resistive MM module for the LPTPC
- Module size: 22 cm × 17 cm
- Readout: 1726 pads, 24 rows
- Pad size: 3 mm × 7 mm



Distortion as observed in *Experiment*
At B=0T. Correction for misalignment has been carried out.

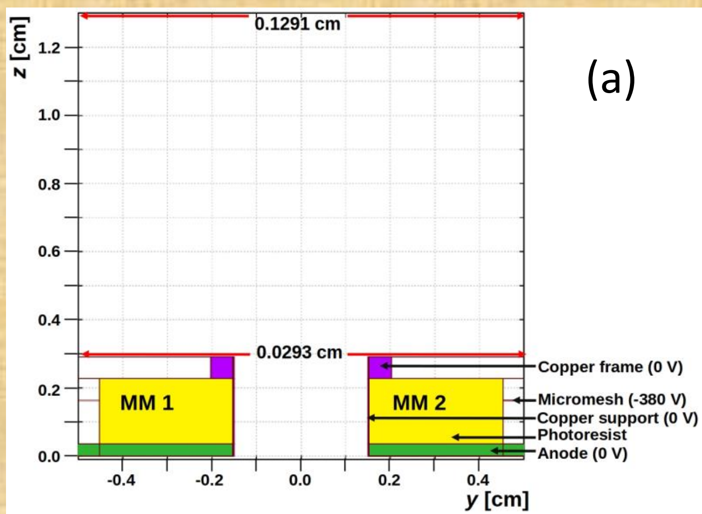


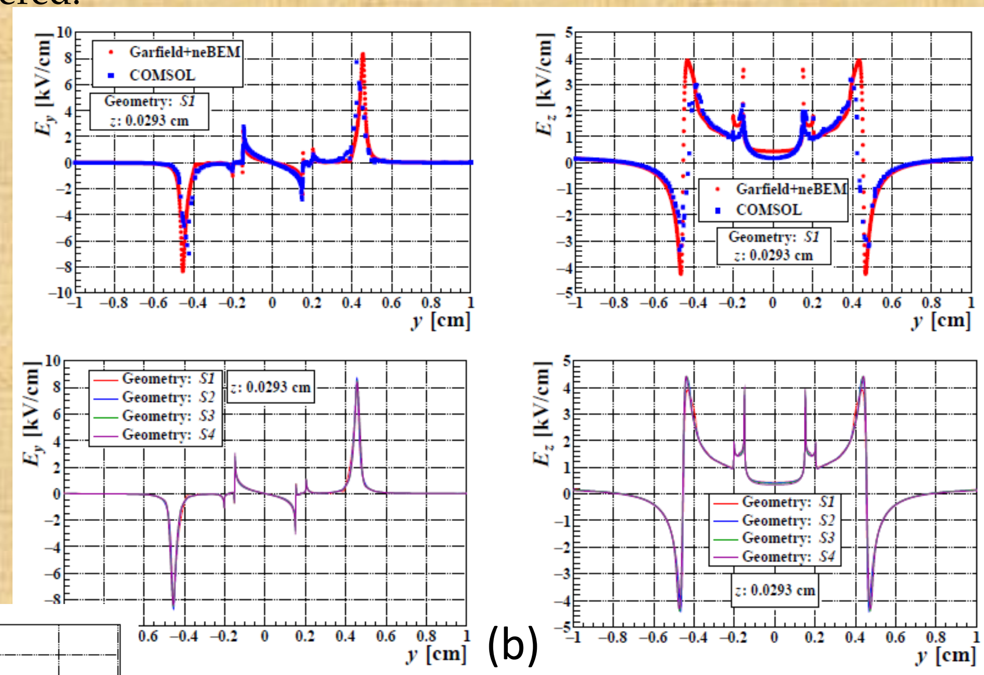
Distortion as observed in *Experiment*
at B=1T. (no alignment correction)

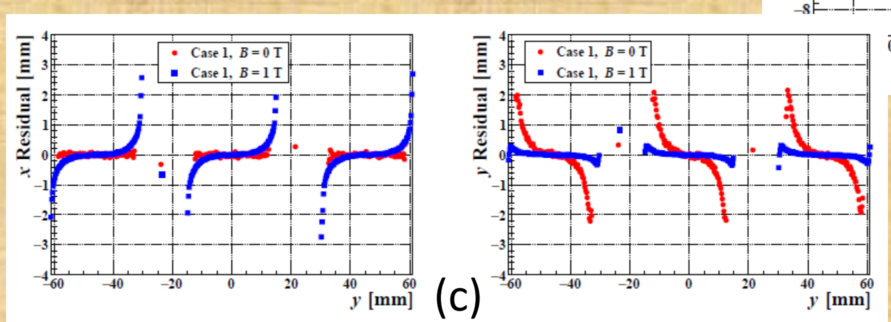
Track is a 5 GeV electron beam

Field non-uniformity and distortion

- Extremely difficult problem from the point of view of field solutions:
  - The component lengths span over several orders of magnitude. For example, length of a module is 22 cm whereas the copper frame width is 30 μm (7000:1). The situation is even worse if the entire device is considered.



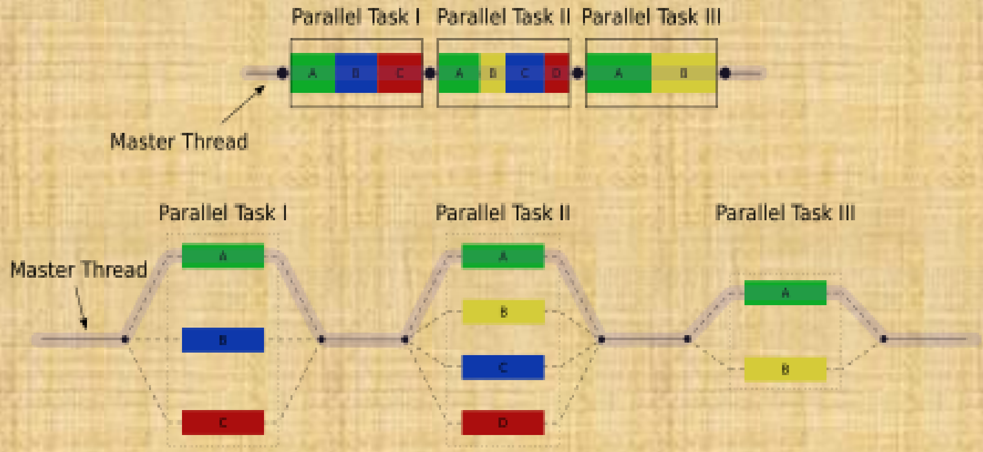


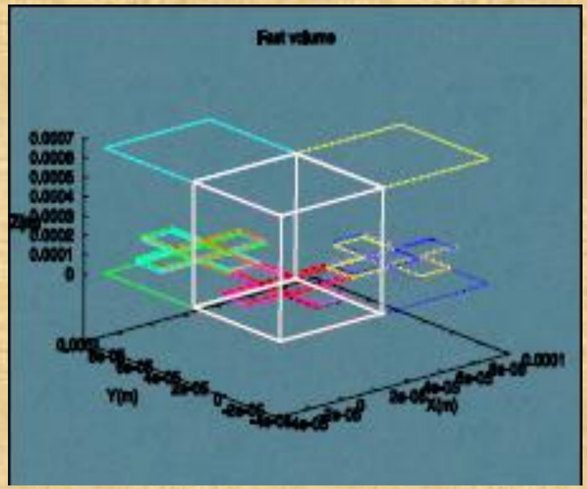


For the B = 0 T case, distortion in both the cases are found to be around 0.5 mm, while for the B = 1 T case, the distortions are around 2 mm. Thus, the estimates are qualitatively and quantitatively comparable to the experimental results.

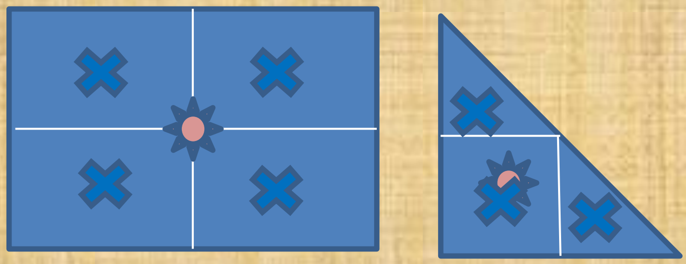
Code Parallelization, Fast Volume, Adaptive Modelling

- Open Multi-Processing (OpenMP): an Application Programming Interface (API).
- Fast volume for both physical and weighting field
- Adaptive modelling / reduced-order modeling: *Can we ignore the variation of charge density on a virtual GEM that is far away from the base device?*





neBEM ongoing developments



- Error estimation: boundary condition being evaluated at non collocation points (can lead to more effective and automatic adaptive meshing)
- Geometry modeler: Geant4 approach
- Charging up: charged particles anywhere in the detector volume can be included; they can also be assigned to elements on which they get deposited
- Space charge: basics are ready
- Charge dispersion: in slow progress

Interface to Garfield++:
To be discussed by Heinrich Schindler in WG4 session

Charging up, dispersion and space charge simulation are extremely resource hungry

Advantages and disadvantages of BEM

advantages	*disadvantages*
• discretization of the boundary only • simplified pre-processing, e.g., data input from CAD can be discretized directly • improved accuracy for secondary variables, e.g., stresses • simple and accurate modelling of problems involving infinite and semi-infinite domains • simplified treatment of symmetrical problems (no discretization needed in the plane of symmetry)	• non-symmetric, fully populated system of equations in collocation BEM • difficult treatment of inhomogeneous and non-linear problems • requires the knowledge of a suitable fundamental solution • practical application relatively recent, not as well known as FEM among users

Summary

- The Boundary Element Method has been introduced.
- Derivation of the Boundary Integral Equation from the original Partial Differential Equation has been demonstrated for the Poisson's equation.
- The procedure of deriving Green's function has been mentioned.
- Conventional single point Collocation method has been illustrated using simple example.
- The nearly exact BEM has been introduced
- The advantages of using neBEM have been demonstrated
- Merits and demerits of BEM have been mentioned.

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Beyond SINP: Rob Veenhof, Heinrich Schindler and members of the RD51 collaboration

Thanks a lot!