Surface Field Calculations for Microscopic Defects

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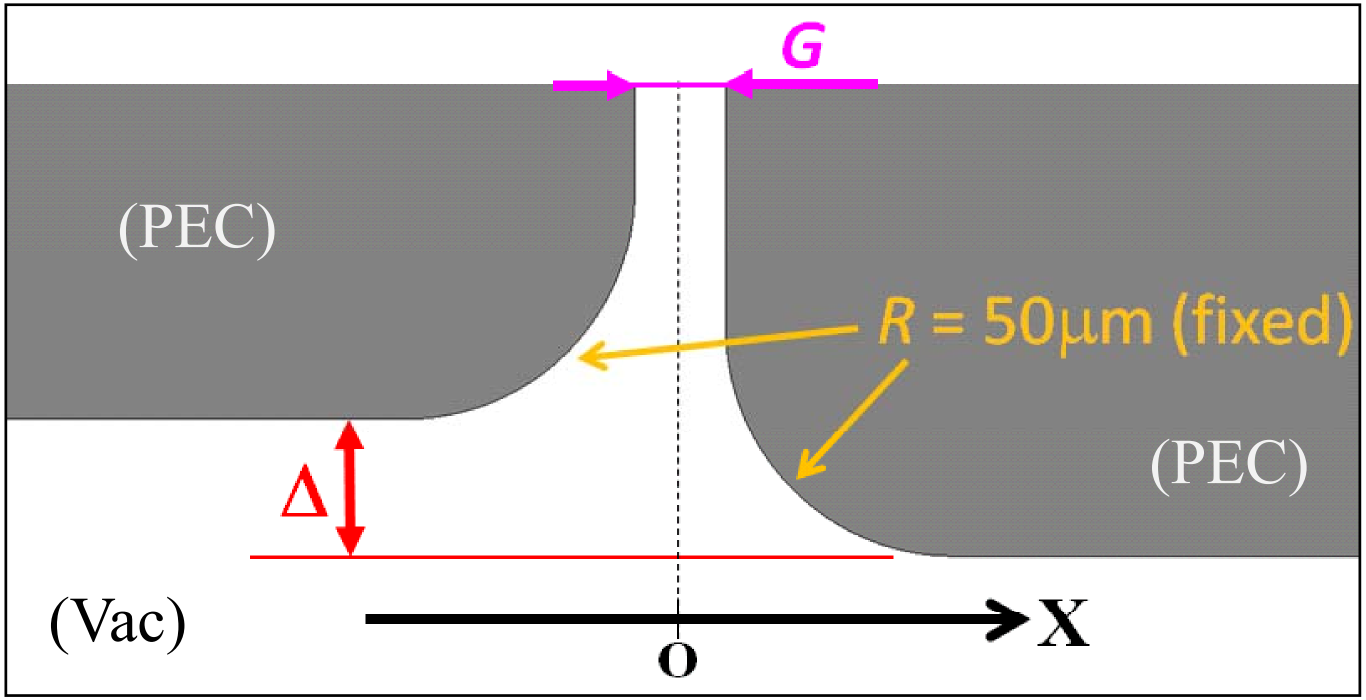
Introduction

- **Microscopic defects**
  →E.g. burrs from machining, undulations due to crystal structures
  →Can be created in accelerating structures
  →Local surface-field enhancements
  →Breakdown trigger of accelerating structures
  →Deterioration of accelerator performance
- **Accurate calculations of such surface fields desired**
- **Concave structure** studied
  - We know: projection tips → Large field enhancements
  - On the other hand, how large enhancements about concave structures?
- **Field enhancement factors** calculated using **three different methods**:
  - Method_1: RF-field simulation based on the Finite Integration Technique (FIT)
  - Method_2: Static-field simulation based on the FIT
  - Method_3: Floating Random Walk

(The FIT is a generalized finite-difference scheme for solving Maxwell's equations, implemented in CST STUDIO SUITE.)

Parameterization of Concave Geometry



PEC: Perfect Electric Conductor (σ = infinite)
Vac: Vacuum

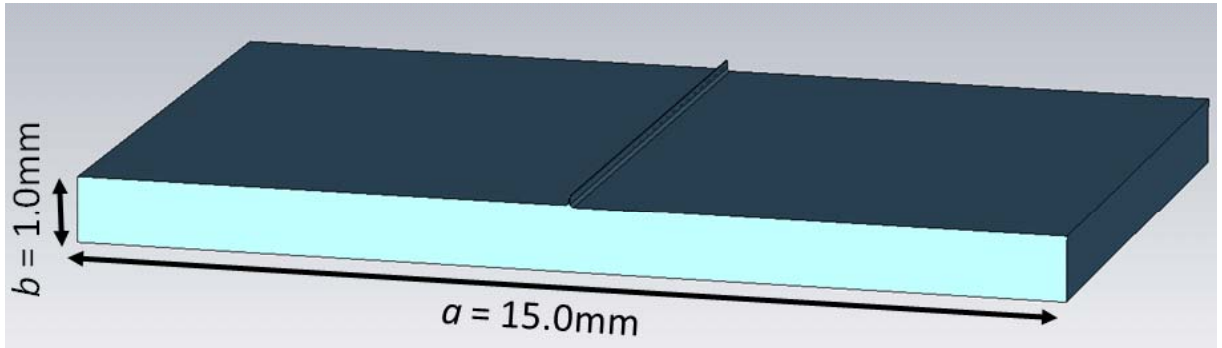
Simulating the round chamfer of the edges of the bonded planes of the Quadrant-type X-band accelerating structure:

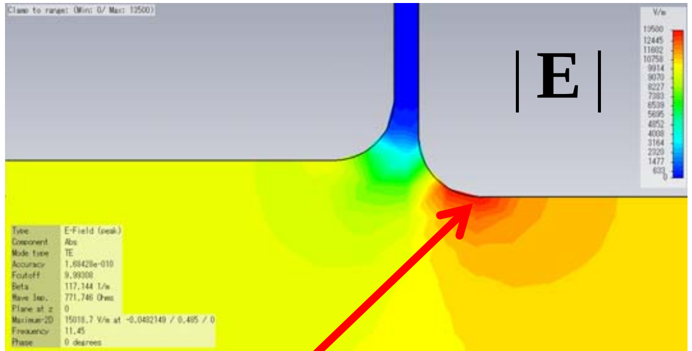
Method_1 : FIT-based RF-Field Simulation using CST Microwave Studio (CST-MWS)

- ✓Rectangular Waveguide with $f_{cutoff}(TE_{10})$ = 10 GHz
- ✓A small groove at the center of the E-plane
- ✓Port mode computation of TE_{10}
- ✓Hexahedral meshing with the PBA

(PBA: Perfect Boundary Approximation)

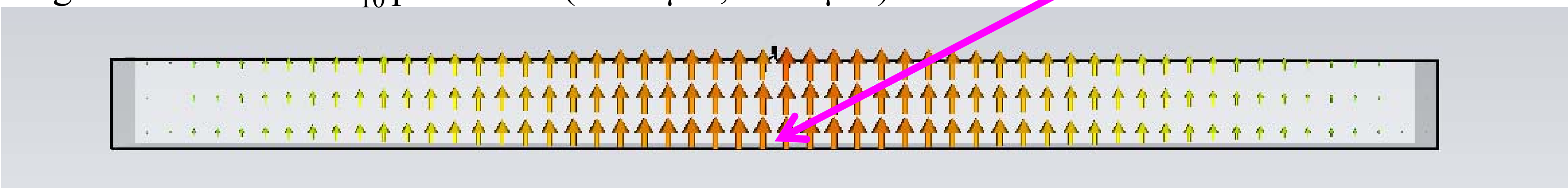
e.g. G=20μm, Δ=30μm





$$\text{Enhancement Factor} \cong \frac{E_{max}}{E_{ref}}$$

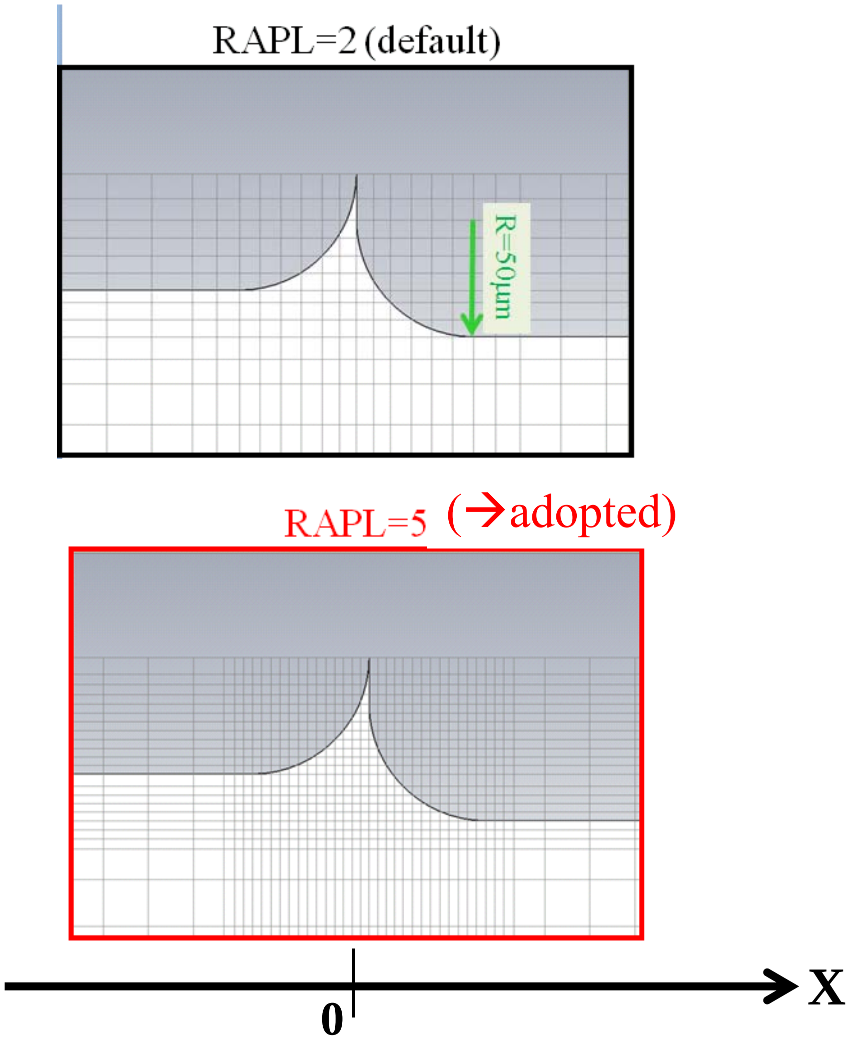
E.g. E-field of the TE_{10} port mode (G=20μm, Δ=30μm):

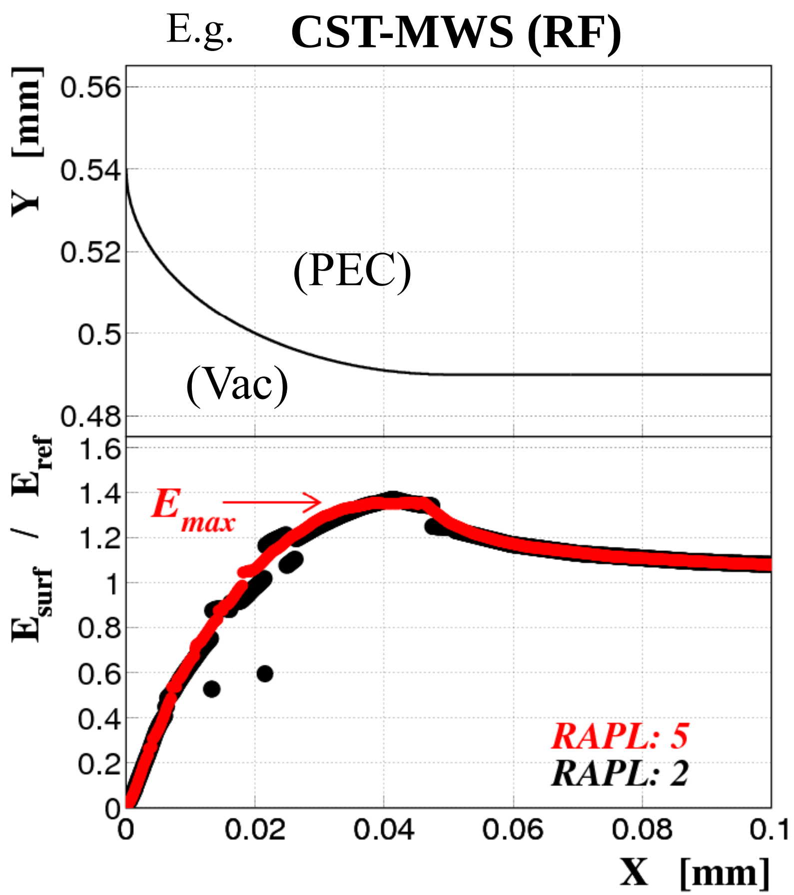


Meshing Parameters and Mesh-Size Dependence

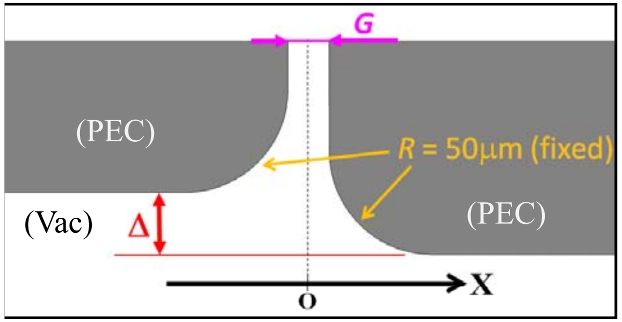
- ✓FDSolver.Method "Hexahedral Mesh"
- ✓Mesh.MeshType "PBA" ‘(Perfect Boundary Approx.)
- ✓**Mesh.LinesPerWavelength “300"** (←10(default))
- ✓Mesh.AutomeshRefineAtPecLines "True", “**RAPL**"
- ✓FDSolver.AccuracyHex "1e-6“

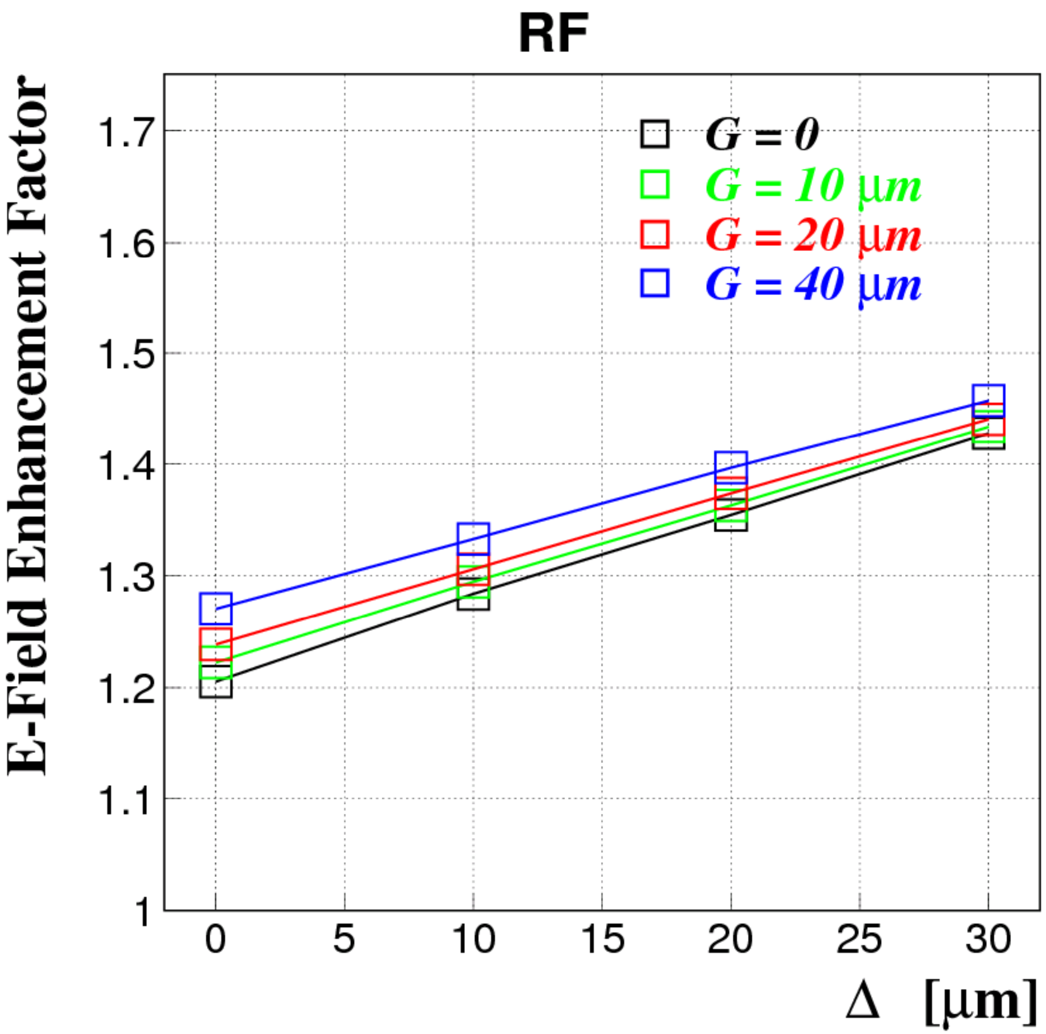
Using a function: “GetFieldVectorSurface()”
→ Better field interpolation scheme on PEC surfaces





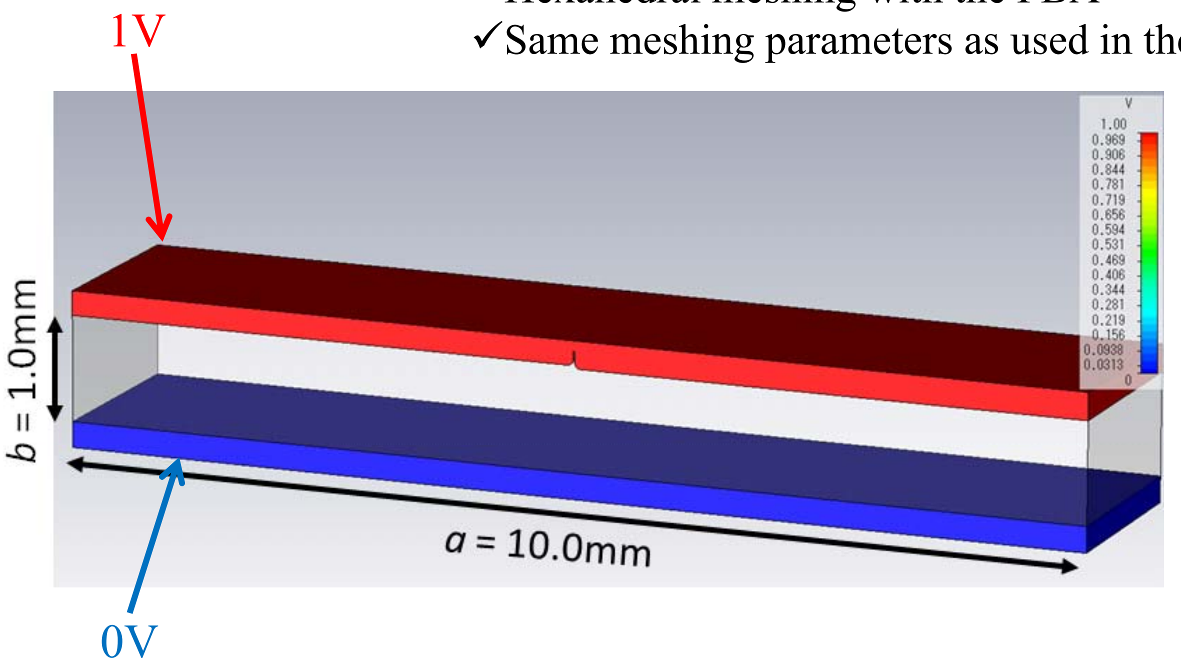
Results by Method_1

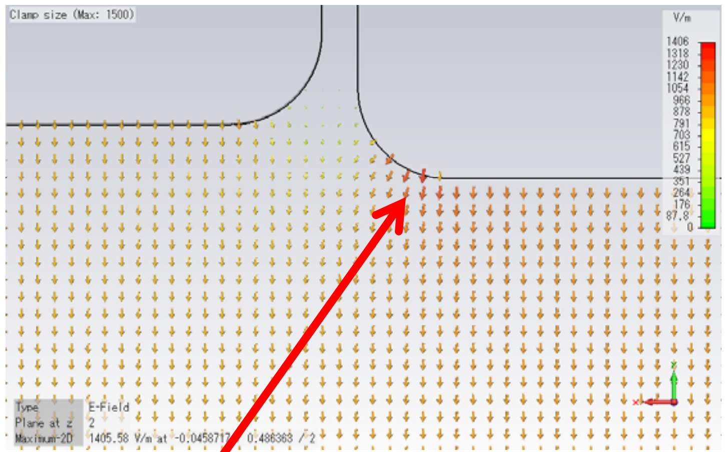




Method_2: FIT-based *Static-Field* Simulation using CST EM Studio (CST-EMS)

✓Static-field approximation
✓Two parallel PEC plates with a small groove (PEC: Perfect Electric Conductor (σ = infinite))
✓Potential difference: 1V
✓Hexahedral meshing with the PBA (PBA: Perfect Boundary Approximation)
✓Same meshing parameters as used in the previous simulation

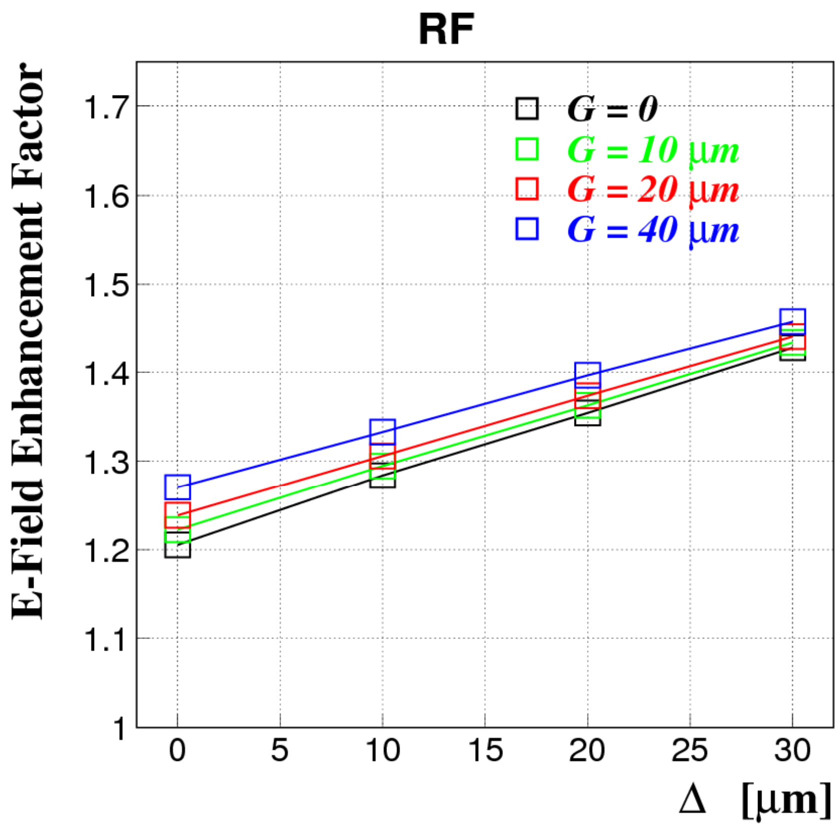


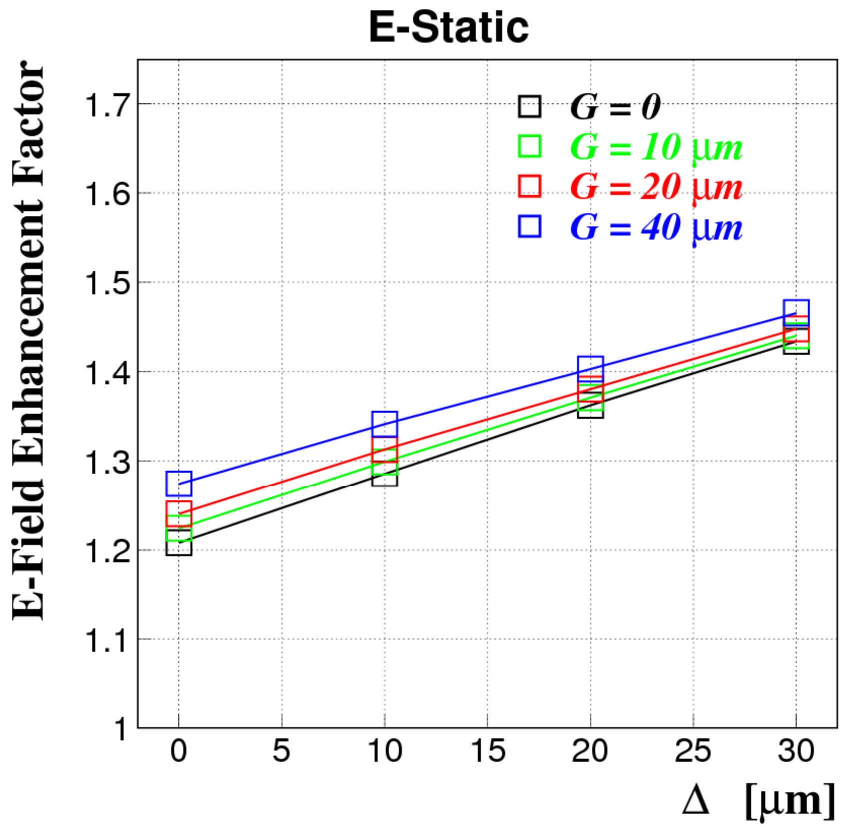


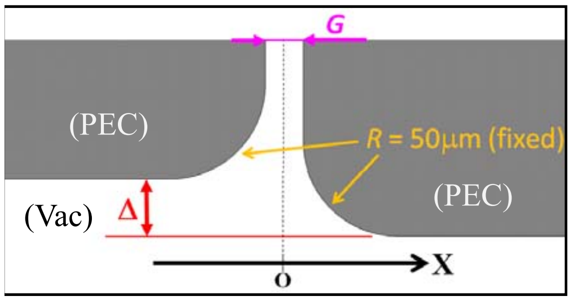
e.g. G=20μm, Δ=30μm

$$\text{Enhancement Factor} = \frac{E_{max}}{1000[\text{V/m}]}$$

Comparison of the Results







✓Good Agreements

✓Static-field Approximation Holds.

Summary of Method_1&2

- **Surface-field enhancements due to small grooves with round chamfer have been computed by using CST-MWS/EMS.**
  - At least 20% enhancement for R=50μm round chamfer.
  - Increases to 40% enhancement as the Δ size increases to 25μm.
  - Good agreements between the two methods (RF and E-static)

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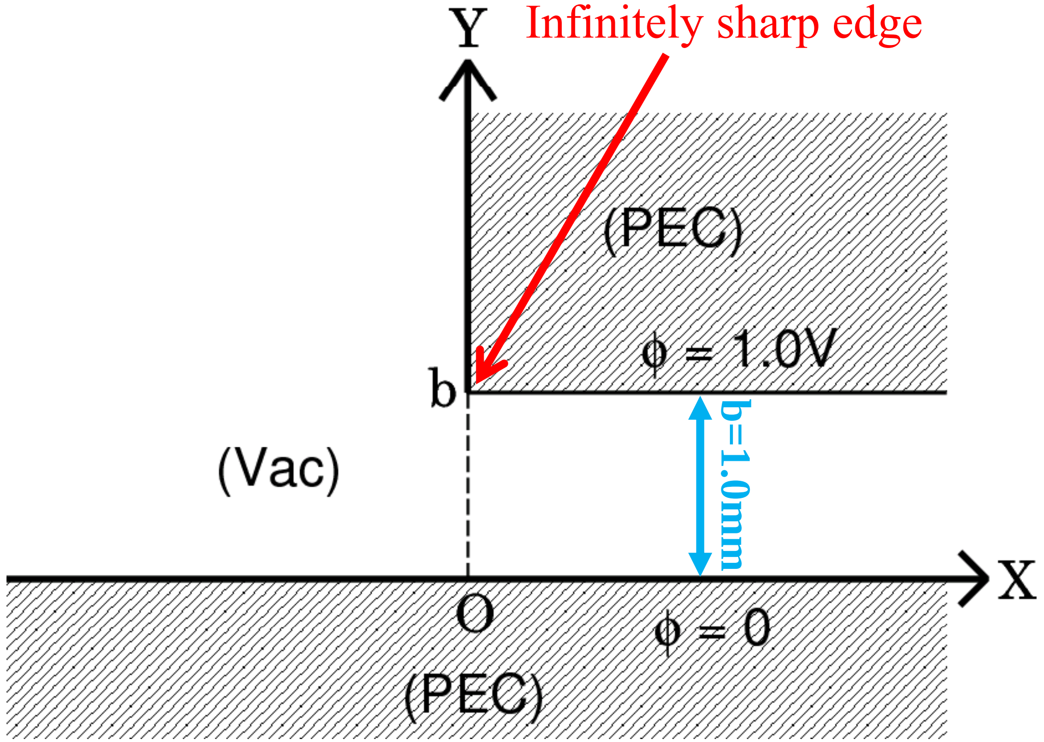
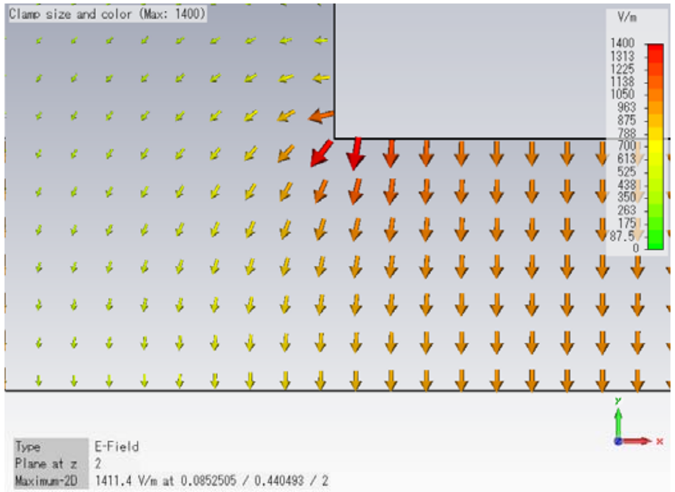
  - Increases to 40% enhancement as the Δ size increases to 25μm.
  - Good agreements between the two methods (RF and E-static)

- **However,**
  - There might be some systematic errors related to the meshing and/or interpolation method.
  - In general,
    - Methods with meshing are week in local-field calculations.
    - It is hard to estimate computation accuracies for finite-element, finite-difference, and finite-integration techniques.
  - Some other methods suitable to local-field calculations?

Benchmark Test



E – Field



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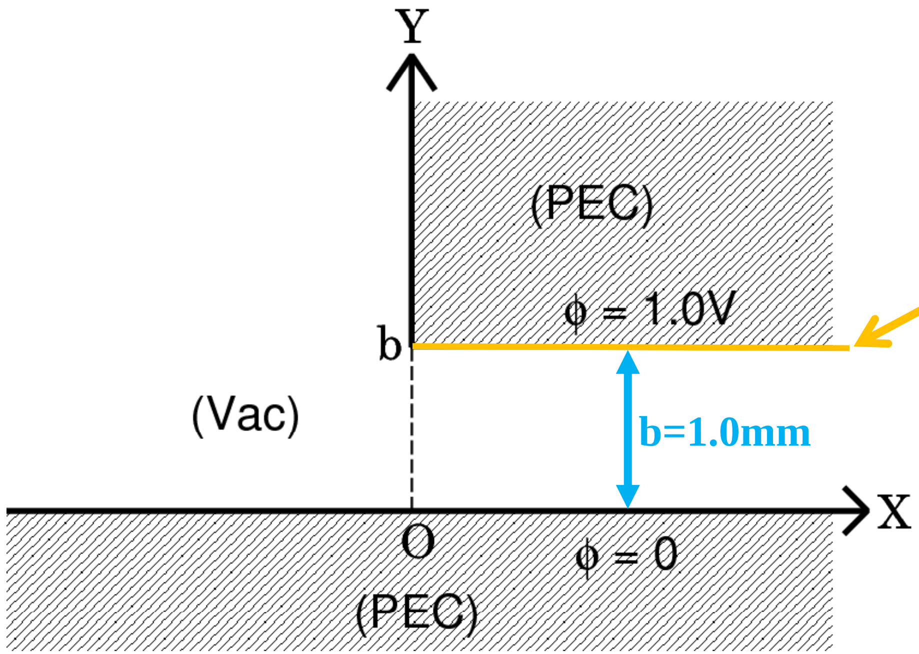
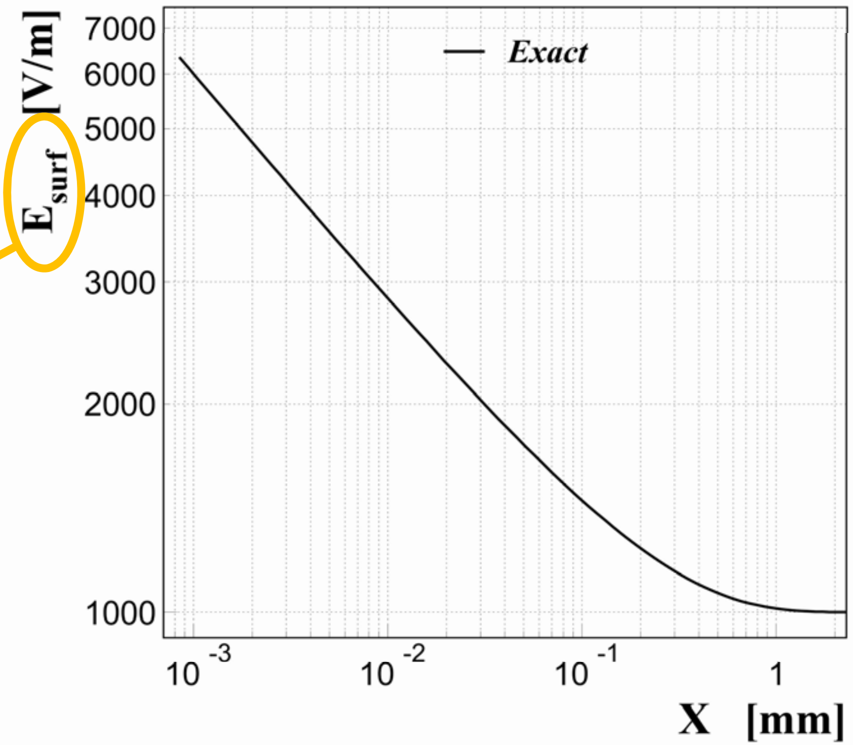
Exact Solution

$$|\vec{E}(X,Y)| = \left|\frac{dw}{dz}\right| \tag{6}$$

From the Schwarz-Christoffel mapping :

$$z = \frac{b}{\pi}\left(\ln\frac{1+\sqrt{1+e^{-(\pi/\phi_0)w}}}{1-\sqrt{1+e^{-(\pi/\phi_0)w}}} - 2\sqrt{1+e^{-(\pi/\phi_0)w}}\right) + ib \tag{7}$$





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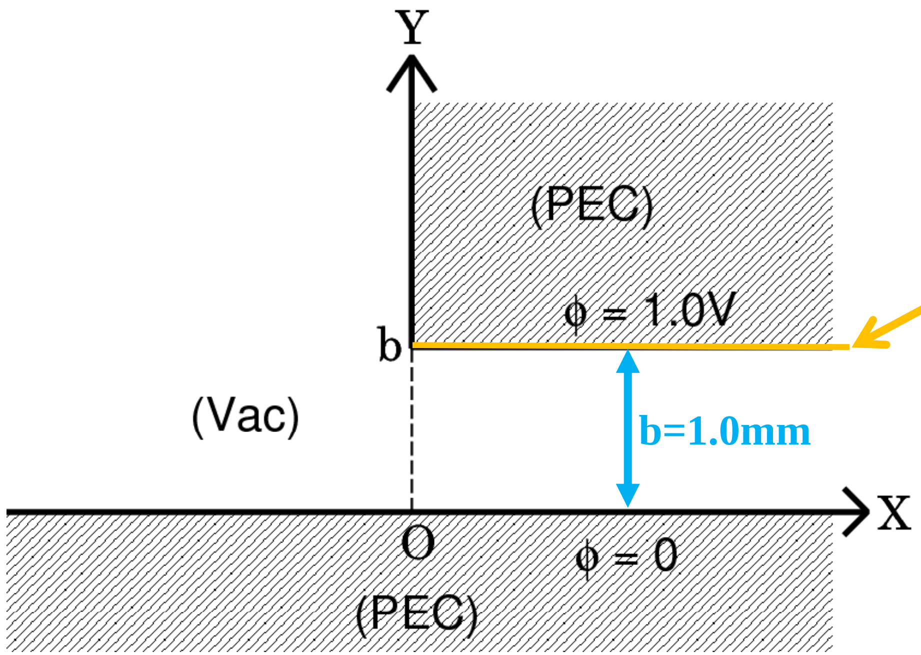
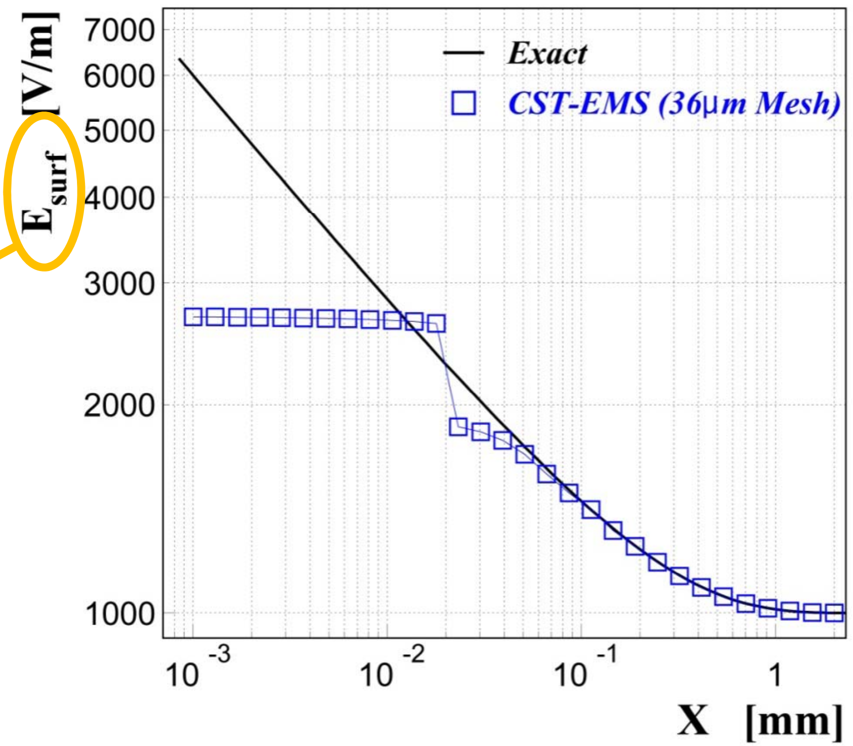
FIT-based Simulation (1)





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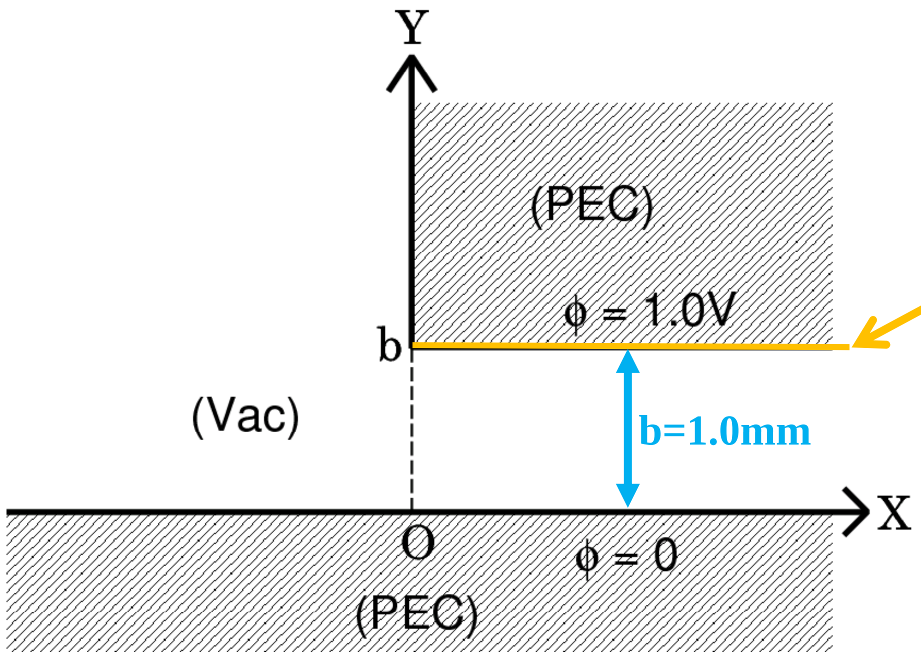
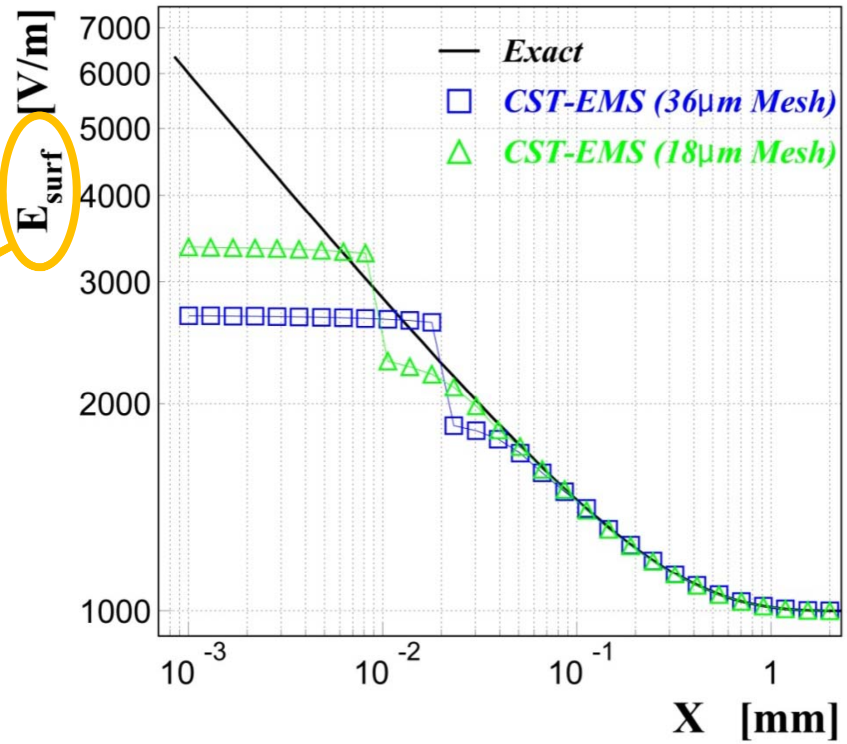
FIB-based Simulation (2)





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Method_3: Floating Random Walk (FRW)

~ A Stochastic Approach ~

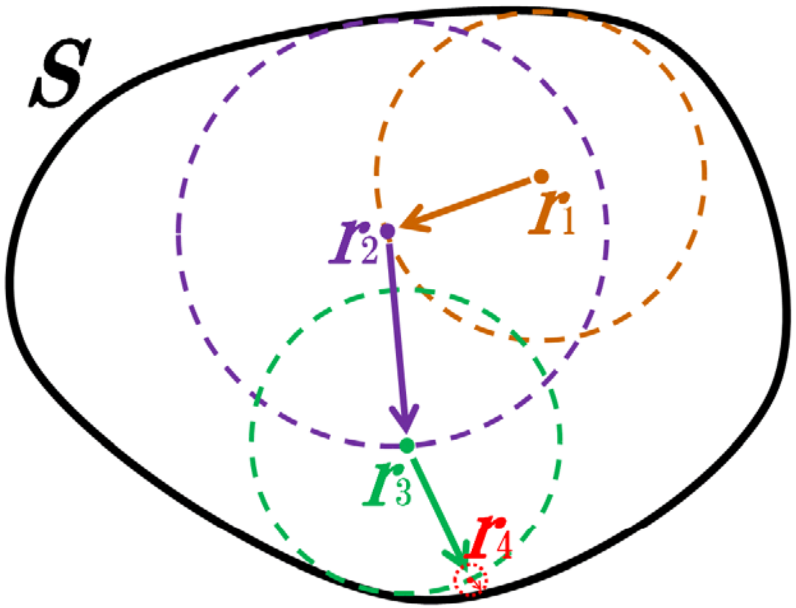
For an electro-static potential ϕ (harmonic function)

$$\begin{aligned}
\phi(X,Y) &= \frac{1}{2\pi r_1}\oint_{C_1} ds_1\, \phi(X_1,Y_1) && (1)\\
&= \frac{1}{2\pi r_1}\oint_{C_1} ds_1 \frac{1}{2\pi r_2}\oint_{C_2} ds_2\, \phi(X_2,Y_2) && (2)\\
&= \frac{1}{2\pi r_1}\oint_{C_1} ds_1 \frac{1}{2\pi r_2}\oint_{C_2} ds_2 \cdots \\
&\qquad \cdots \frac{1}{2\pi r_N}\oint_{C_N} ds_N\, \phi(X_N,Y_N)\,, && (3)
\end{aligned}$$

where C_N indicates a circle with a fixed radius of r_N:

$$r_N = \sqrt{X_N^2 + Y_N^2}\,, \qquad (4)$$

and the value of r_N is always set to be the minimum distance to the boundary with a known potential. In the FRW



The multiple integration (3) can be given a probabilistic interpretation, and estimated by many random walks in a Monte-Carlo method

Method_3: Floating Random Walk (FRW)

Letting ϕ_k be an estimate by the k-th single random walk, and performing M random walks in total, we obtain an estimate $\bar{V}$ and its error σ of the potential by M random walks according to the following formula:

$$\bar{\phi} = \frac{1}{M}\sum_{k=1}^{M}\phi_k \, , \quad \sigma = \frac{\text{(Standard Deviation)}}{\sqrt{M}} \, . \qquad (5)$$

Advantages of FRW

1. No meshing (i.e. no space discretization)
2. Simple algorithm,
3. No large amount of computer memory needed,
4. High parallelization efficiency (← Monte Carlo method)
5. Calculation accuracies also estimated,
6. Higher accuracy with larger statistics of random walks.

Disadvantage of FRW

Larger number of computations or operations are needed than in the deterministic methods, such as finite-element, finite-difference, and finite-integration techniques.

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Larger number of computations or operations are needed than in the deterministic methods, such as finite-element, finite-difference, and finite-integration techniques.

Can be overcome by adopting

GPGPU (General-Purpose computing on Graphics Processing Units)

- *Many cores*
- *Rapidly-advancing field in computer science*

It should be noted that GPGPU is weak in complicated algorithms.

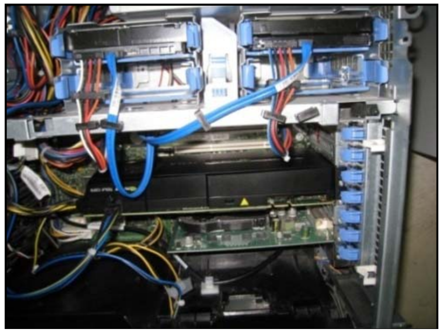
GPGPU Computing

The FRW algorithm to calculate local fields is implemented
in my own computer program for GPGPU
written in CUDA Fortran / Fortran 2003.

This program was executed in a personal computer (<u>Dell Precision T7400</u>)
with a GPGPU board of <u>NVIDIA Tesla C2070</u>.

448 CUDA cores inside

CPU: Quad-core Xeon X5472 (3.0 GHz) x 2



Two Simulation Parameters in FRW

δn

Tiny distance from the conductor surface to compute electric fields:

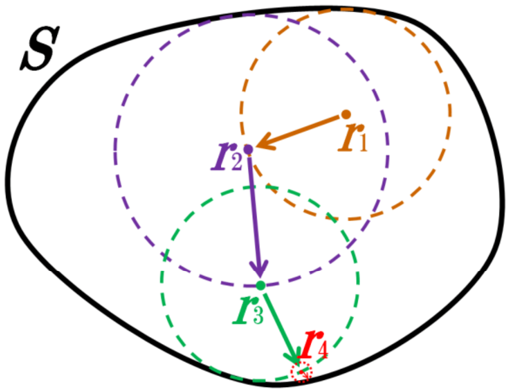
$$E = (\, 1.0V - V_{FRW}(\delta n)\,) \,/\, \delta n$$

$V_{FRW}(\delta n)$: potential at a distance of δn from the conductor surface

r_{min}

Very tiny distance to terminate random walks

e.g

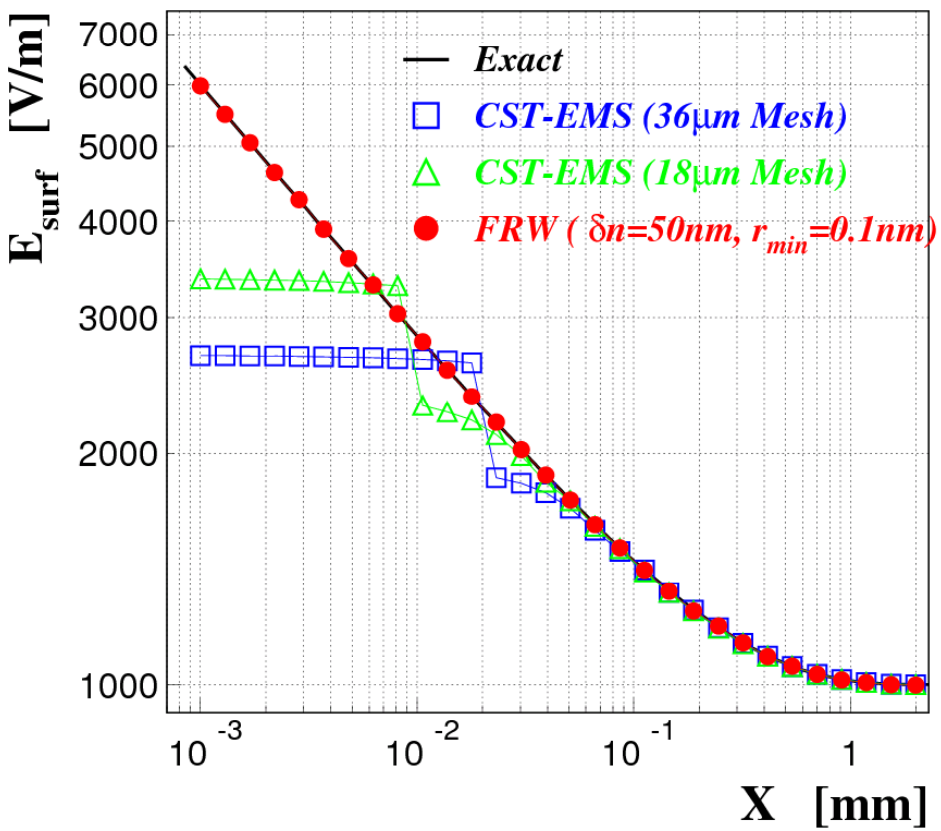


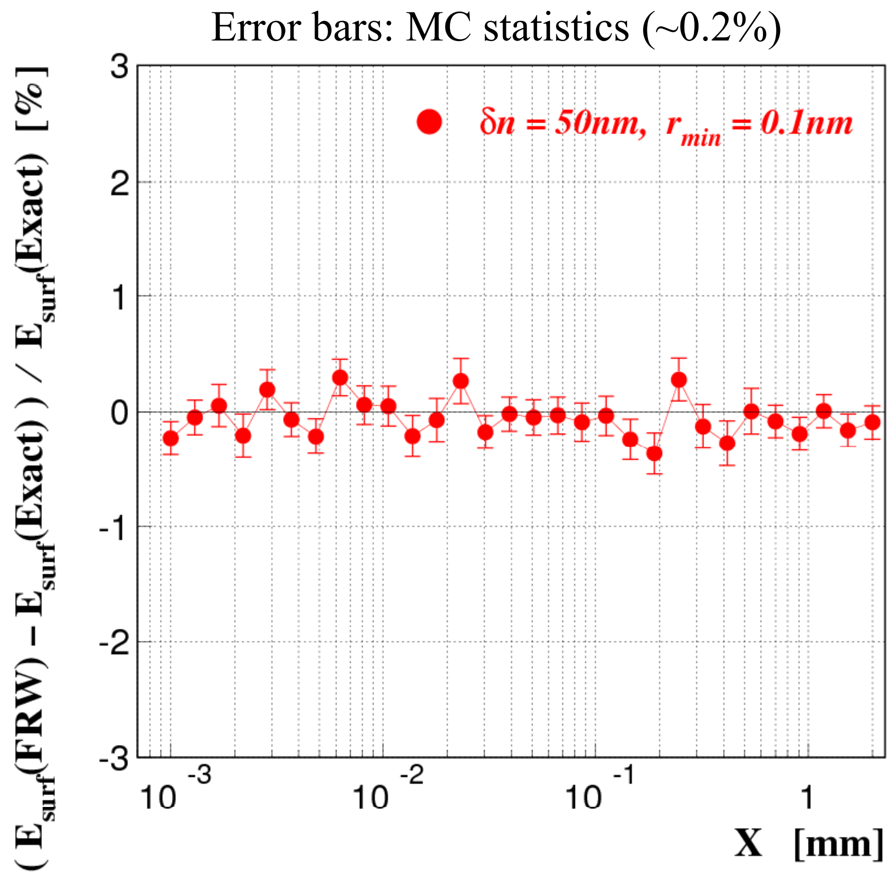
If $r_4 < r_{min}$,

- This random walk terminated
- The potential at the nearest boundary used

How to Determine these Two Parameters ?

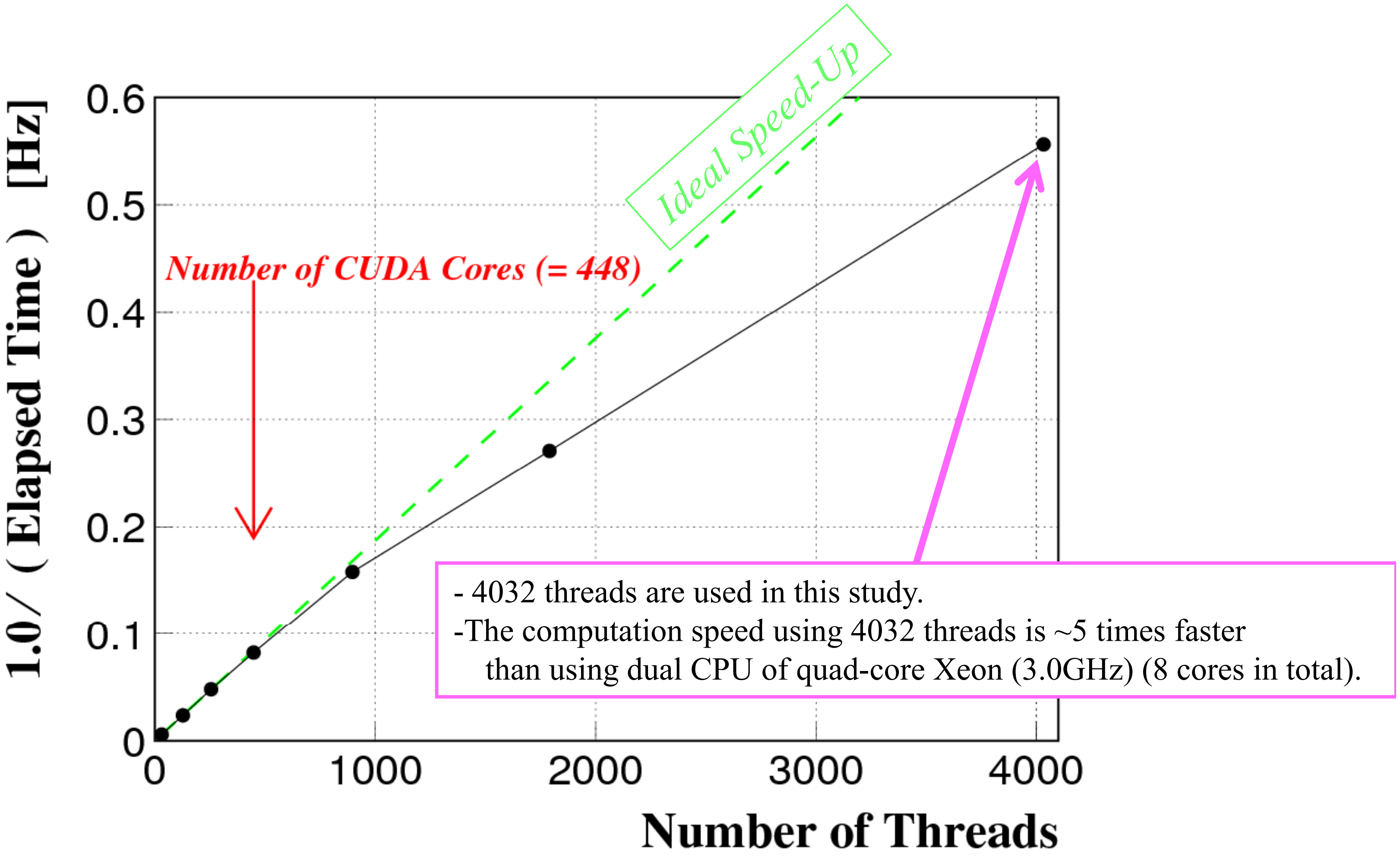
In this study,
(δn, r_{min}) is set to be (50nm, 0.1nm)
*so as to have a **1μm-Resolution** Computational Probe*
for the benchmark test.



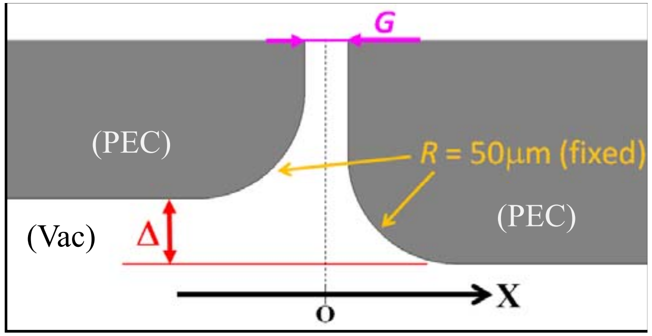


Parallelization Efficiency

For a FRW computation on the benchmark test using one GPGPU board (NVIDIA Tesla C2070)

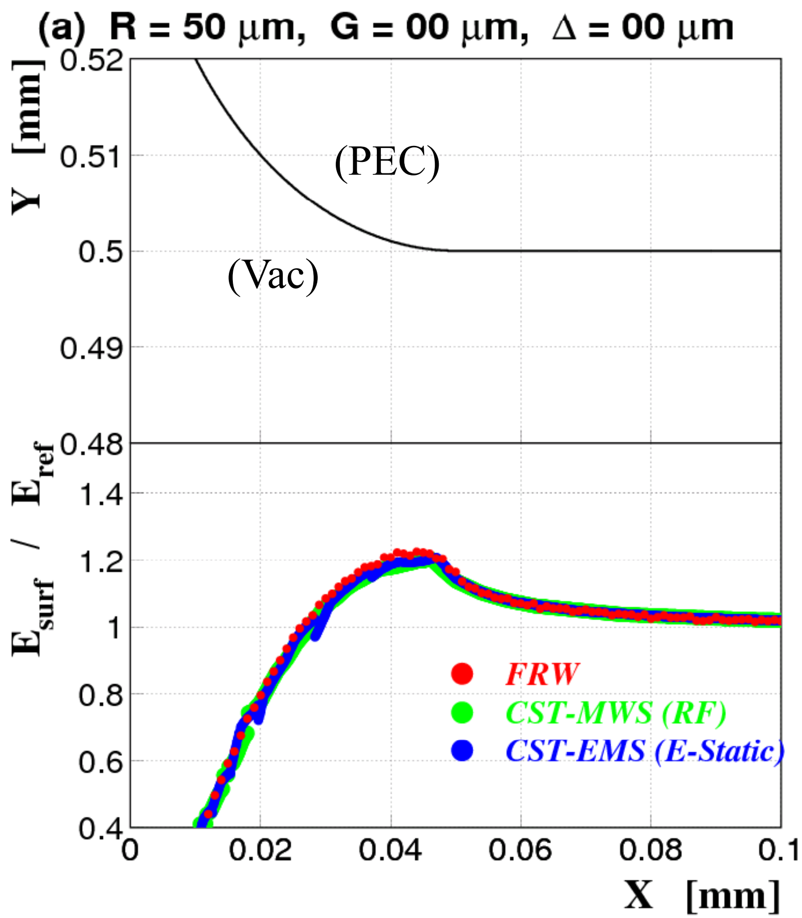


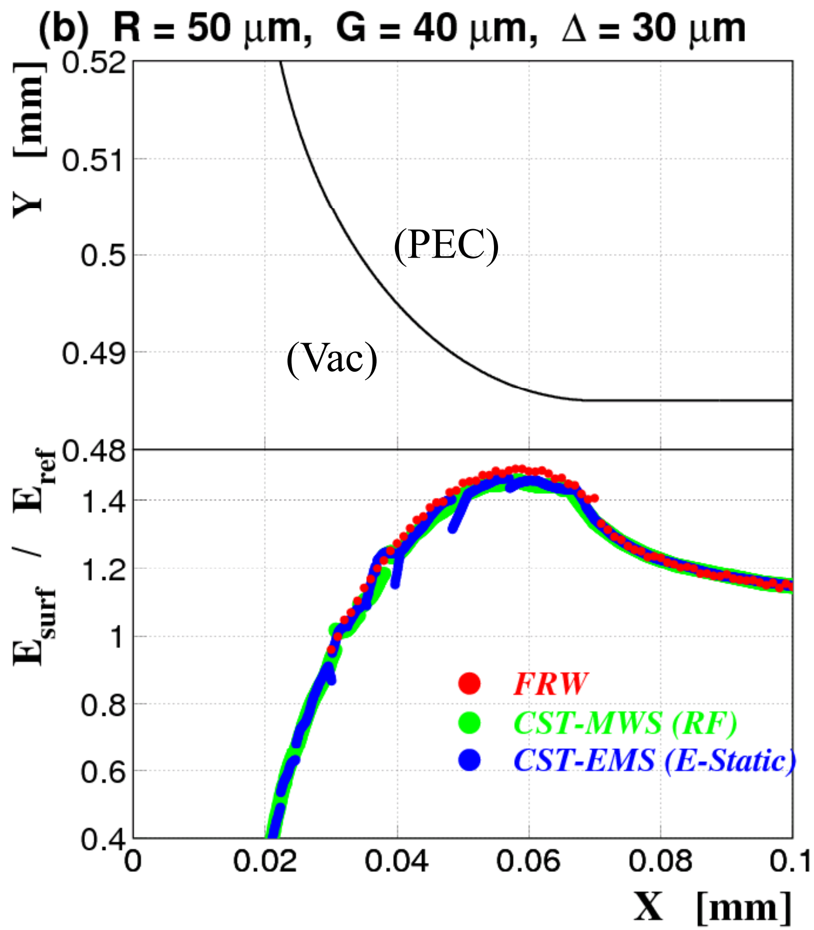
Comparisons with the FIT-based Simulations



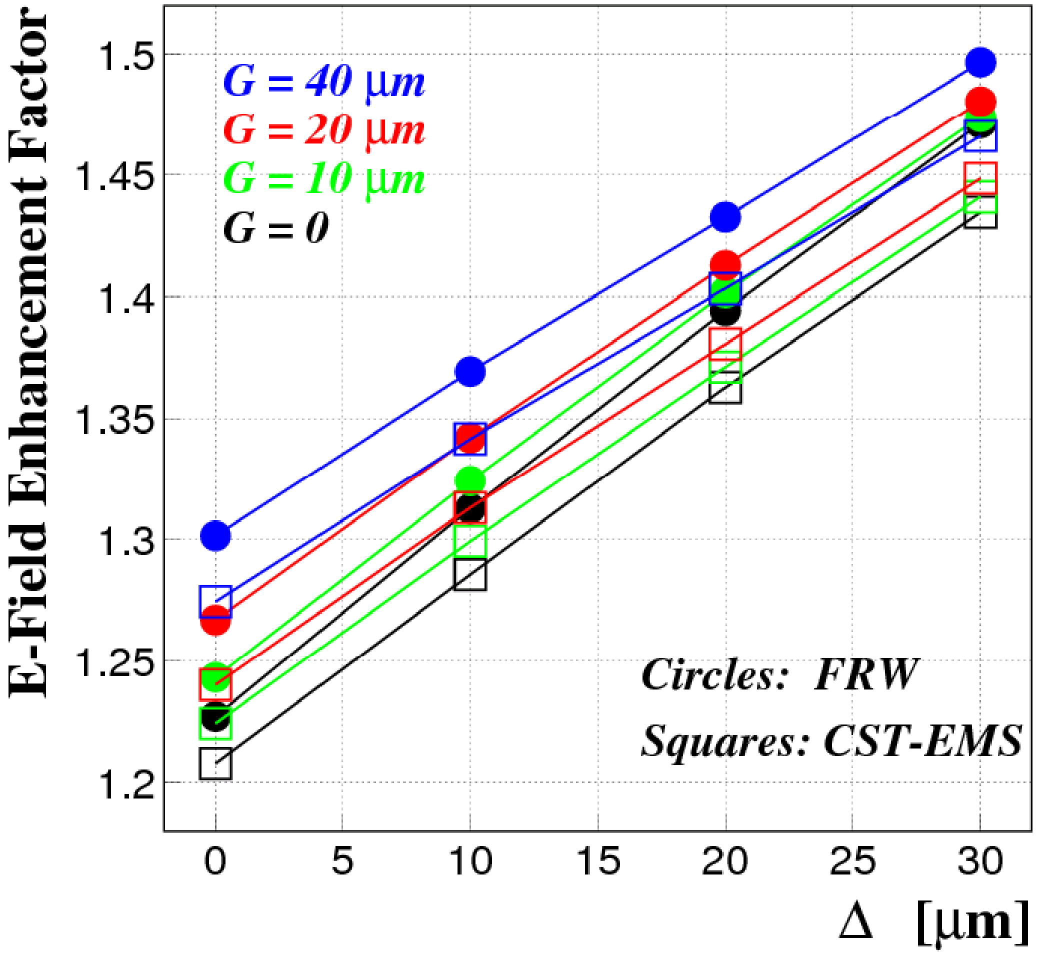
FRW

- ✓MC statistics: ~0.4%
- ✓Number of random walks / point : ~1 billion (=M)
- ✓Elapsed time of computation / point : ~1 minute





Results



- ✓Theoretically the equivalent calculations performed on the FRW and CST-EMS (E-static)
- ✓Systematically a few % smaller by CST-EMS than using the FRW

Conclusions for Method_3 (FRW)

- **It has been found that**
  - The FIT-based simulations using CST-MWS/EMS systematically give a few % lower field-enhancement factors than using the FRW.

- **It has been demonstrated that the FRW method**
  - Can give highly-accurate calculations of local surface fields for microscopic objects,
  - Practical and Promising because of its suitability for GPGPU computing.
    - Significant speed-up to be achieved by further code improvements and using a GPU cluster

      → Better-resolution computational probe

- **This FRW method is applicable to any structures.**
  - Next step: Surface field calculations for real conductor surfaces (3D) damaged by breakdowns/discharges, etc.
  - What kind of shapes makes large field enhancements?

To be Continued...