Simulation of Transition Radiation from a flat target using CST particle studio.

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Motivation

- In accelerator physics research various target geometries such as screens and gratings are used for beam diagnostics.
- Most of these target geometries have well developed analytical models which describe the characteristics of radiations such as Transition, Diffraction and Smith – Purcell radiation.
- These models are usually idealised and not always suitable for comparison with experimental data (edge effects, material properties, surrounding hardware, diffraction and interferometric effects).
- Advanced electromagnetic simulations provide an opportunity to perform simulations describing a real experiment in a more efficient manner.
- THz frequency range in the simulations.

Talk overview

- Overview of the CST particle studio and its solvers.
- Finite Integration Theory.
- Particle In Cell Solver.
- Meshing procedure.
- Beam definition.
- Simulation of Transition Radiation from a flat ideally conducting screen.
- Comparison with the existing theoretical investigations.
- Vision of the future applications for more complex target geometries.

CST Particle Studio

Computer Simulation Technology (CST) Particle Studio (PS) is a specialist tool for the analysis of free moving charged particle dynamics in 3D electromagnetic fields.

Three solvers in the package:

1. Tracking solver.

Tracking in static E/H fields. Simulations of DC Particle Guns, Magnets.

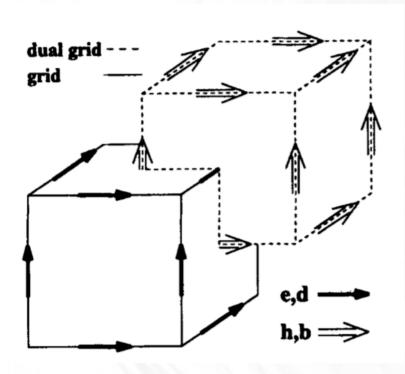
2. Particle in Cell solver.

Self-consistent transient field and particle solver, including space charge effects. Simulations of MW tubes (Traveling Wave Tube, Klystron...)

3. Wakefield solver.

Transient solver with special beam excitation (predefined fixed straight beam path).

Finite Integration Approximation



Non-co-ordinate grids are introduced to improve the capability of a grid to approximate curved boundaries.

Maxwell-Grid-Equations are defined on a dual grid doublet $\{G,\widetilde{G}\}$

$$\iint_{A} -\frac{\partial}{\partial t} \mathbf{B} \cdot d\mathbf{A} = \oint_{\partial A} \mathbf{E} \cdot d\mathbf{r} -\frac{\partial}{\partial t} \mathbf{b} = \mathbf{C} \mathbf{e}$$

$$\iint_{\partial V} \mathbf{B} \cdot d\mathbf{A} = 0 \qquad \mathbf{S} \mathbf{b} = \mathbf{0}$$

$$\iint_{A} \left(\mathbf{J} + \frac{\partial}{\partial t} \mathbf{D} \right) \cdot d\widetilde{\mathbf{A}} = \oint_{\partial \widetilde{A}} \mathbf{H} \cdot d\widetilde{\mathbf{r}} \qquad \mathbf{j} + \frac{\partial}{\partial t} \mathbf{d} = \widetilde{\mathbf{C}} \mathbf{h}$$

$$\iint_{A} \mathbf{D} \cdot d\widetilde{\mathbf{A}} = \iiint_{V} \rho d\widetilde{V} \qquad \widetilde{\mathbf{S}} \mathbf{d} = \mathbf{q}$$

- e, h are electric and magnetic grid voltage vectors.
- d, j, b are facet flux vectors.

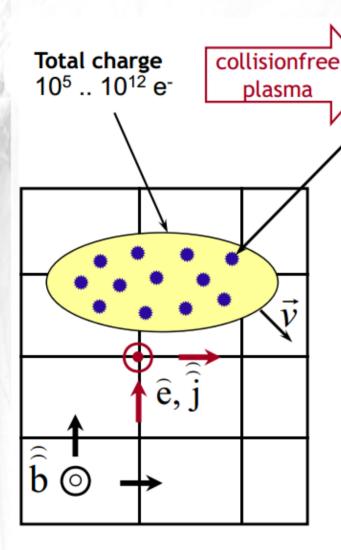
Discrete permeability, permittivity and conductivity are defined as:

$$\mathbf{b} = \mathbf{D}_{\mu}\mathbf{h}; \quad \mathbf{d} = \mathbf{D}_{\varepsilon}\mathbf{e}; \quad \mathbf{j} = \mathbf{D}_{k}\mathbf{e}$$

 $\mathbf{D}_{\mu}, \mathbf{D}_{\varepsilon}, \mathbf{D}_{k}$ are material matrices (diagonal for dual orthogonal grid-doublets).

*T. Weiland, Time domain electromagnetic field computation with finite difference method, International Journal of Numerical Modelling: Electronic networks, Devices and fields, Vol. 9, 295-319 (1996).

Particle in Cell (PIC) Algorithm



Macro charges (e.g. Q=10⁶ e⁻)



 Number e⁻ / macroparticle individual different

Relativistic equation of motion

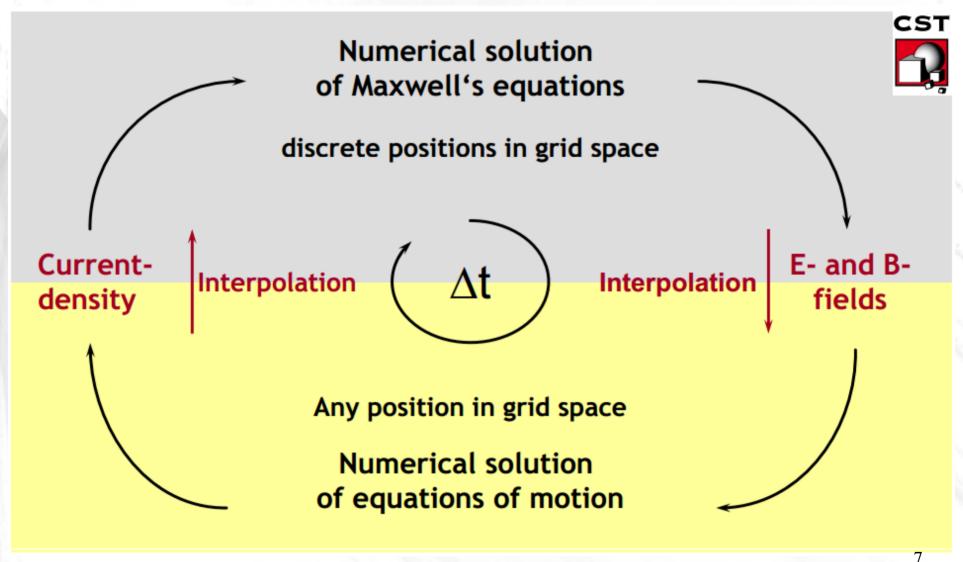
$$\frac{\partial \vec{u}}{\partial t} = \frac{q}{m_0 c} \left(\vec{E} + \vec{v} \times \vec{B} \right)$$

$$\frac{\partial \vec{r}}{\partial t} = \vec{v} \qquad \vec{u} = \frac{\vec{p}}{m_0 c} = \frac{m(v)\vec{v}}{m_0 c} = \gamma \cdot \vec{\beta}$$

Feedback of particle motion via an a priori charge conserving current scheme

$$\operatorname{rot} \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}; \qquad \operatorname{div} \vec{J} = -\frac{\partial \rho}{\partial t}$$

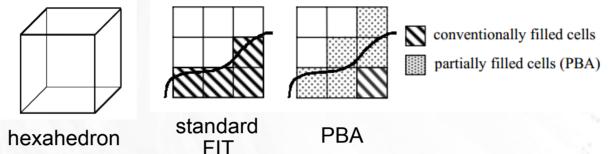
Particle in Cell (PIC) Algorithm



Meshing procedure

For the spatial discretisation the <u>Finite Integration Technique (FIT)</u> in conjunction with the <u>Perfect Boundary Approximation (PBA)</u> is used.

A simulated structure and electromagnetic fields are mapped to hexagonal mesh.



PBA allows for a very good approximation of even curved surfaces with the cubic mesh cells. Sub-cellular information is taken into account, leading to an algorithm with the second order accuracy.

Options for meshing:

Automatic

(An expert system automatically chooses the best PBA for optimal performance and accuracy)

Manual

(PBA and Staircase mode)

Tweaking:

Adaptive mesh refinement (creation of fix-points and density-points)

Mesh refinement at Perfect Electric Conductor edges

Lines per wavelength (defines the minimum number of mesh lines per wavelength)

Lower mesh limit (defines the maximum mesh step),

Ratio limit (defines the ratio between the biggest and smallest distance between mesh lines).

Particle Source definition

A particle beam is defined as a point like source (in the transverse direction) which enters the calculation domain at a certain position and propagates with constant velocity along the straight

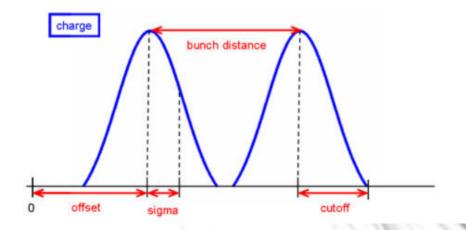
line.

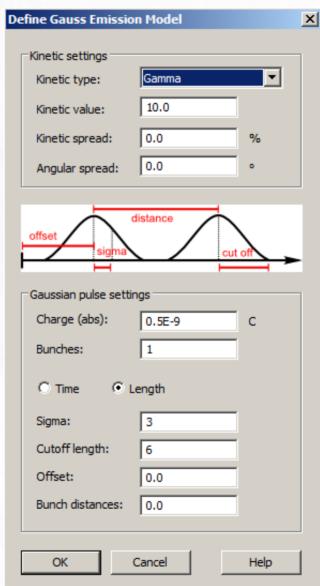
The charge distribution as a function of the longitudinal coordinate **s** is defined as follows:

$$q(s) = q_{total} \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{s^2}{2\sigma^2}\right)$$

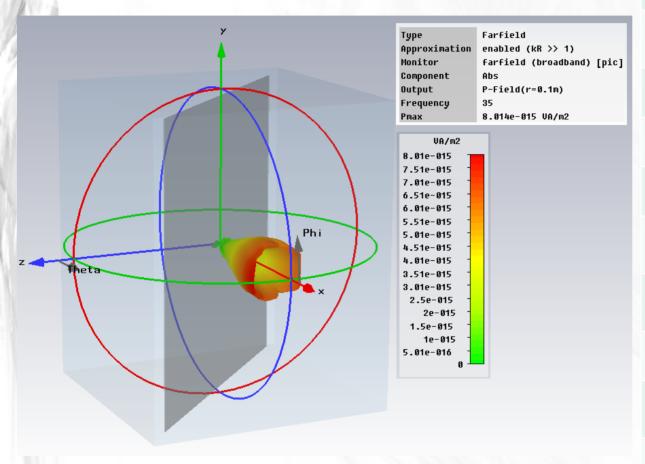
Gauss emission model can be considered for a point like source or a circular type source where the charge is uniformly distributed over the emission area.







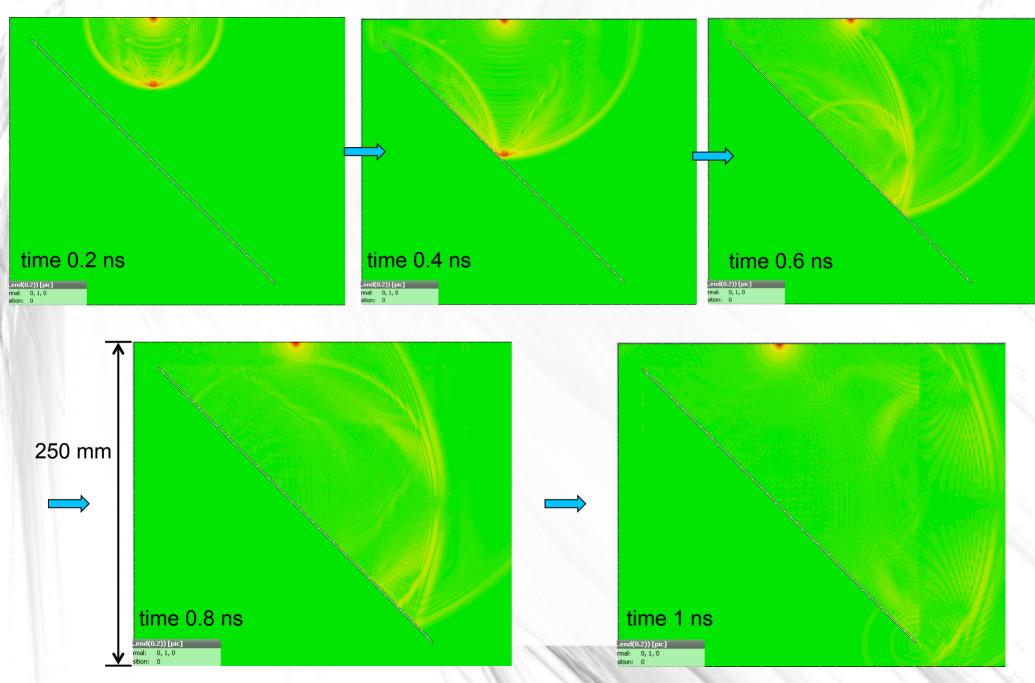
Model description



Boundaries are open	(act as free space))
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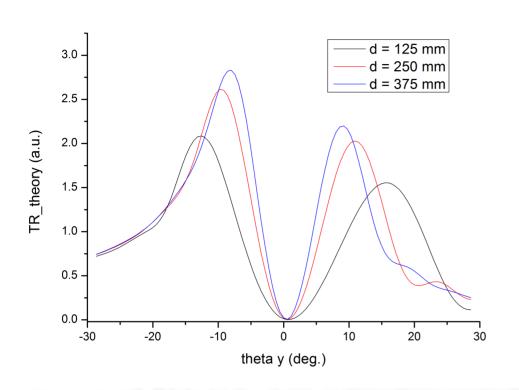
Parameter	Value
gamma (γ)	10 (5 MeV)
frequency (wavelength)	25 GHz (12 mm)
target dimensions	150x150 mm
target thickness	1 mm
target material	PEC
target inclination angle	45 deg.
σ of longitudinal charge distribution	0.03 mm
bunch charge	0.5 nC
Volume xyz	L x 310 x 250 mm
L	250/375/500 mm

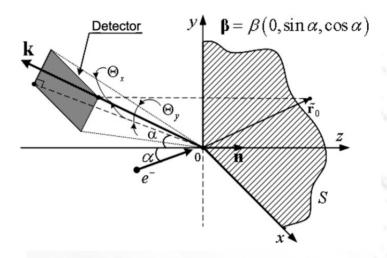
Charge / TR propagation



THz workshop during RREPS13, Meghri13, Yerevan, 23-27 September 2013

Theoretical model

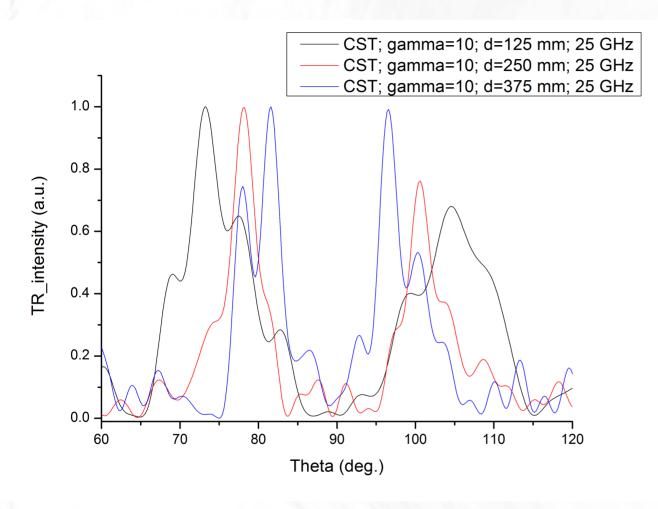


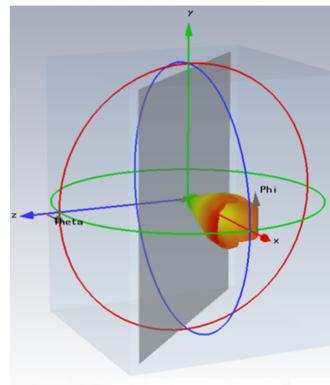


$$\gamma = 10; \lambda = 12 \, mm; \alpha = 45 \, deg.$$

For comparison with CST simulations the theory developed by D.V. Karlovets and A. P. Potylitsyn for Transition Radiation in the pre-wave zone for an oblique incidence of a charged particle on the flat target was used.

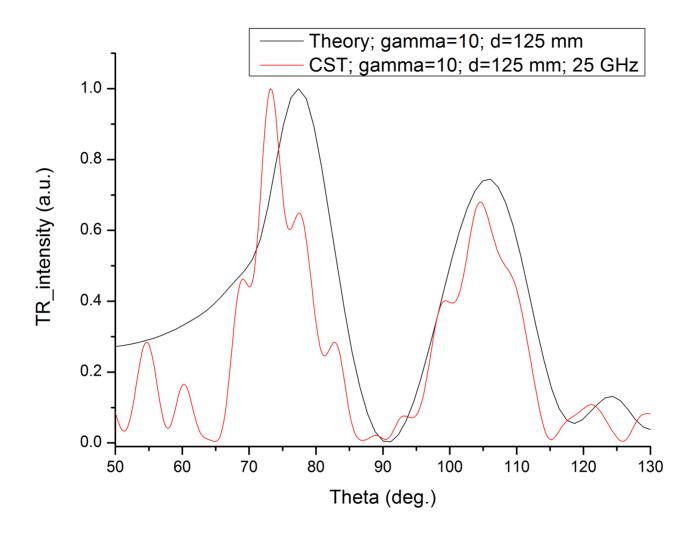
*D.V. Karlovets, A.P. Potylitsyn, NIMB 266 (2008) 3738-3743.



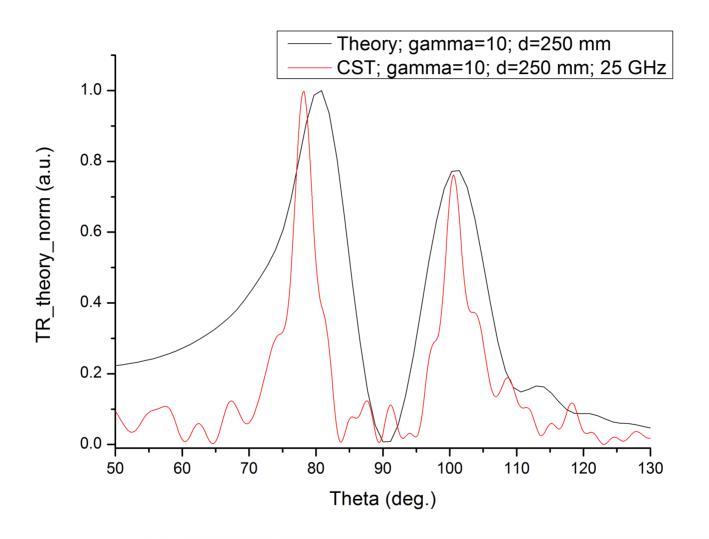


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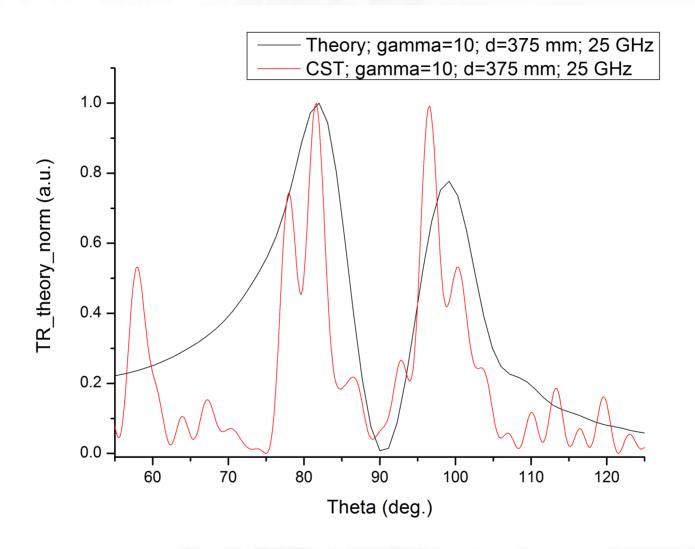
TR distributions in the horizontal plane (Phi = 0 deg.; Theta = 60 - 120 deg.)



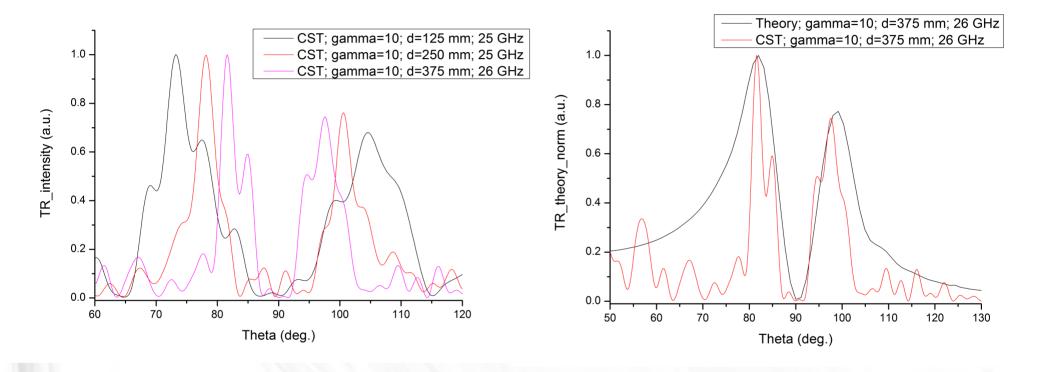
Comparison of the theoretical distribution in the pre-wave zone with the simulated distribution for d = 125 mm.



Comparison of the theoretical distribution in the pre-wave zone with the simulated distribution for d = 250 mm.



Comparison of the theoretical distribution in the pre-wave zone with the simulated distribution for d = 375 mm.



Now slightly different frequency (26 GHz) for d = 375 mm is chosen, better agreement is demonstrated (simulation stability issue).

Summary and Outlook

As yet the simulations were performed in the context of studying the capabilities of CST for calculation of the TR, that has been studied analytically and is well understood phenomenon.

Simulation performance:

- calculation stability;
- correct meshing and adaptive meshing optimisation;
- establish communication with CST experts to receive qualified and expert advise on the types of solvers and other parameters to be used.

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General outlook:

- the main goal is to establish accurate and reliable tool for numeric calculations of irradiative processes used for THz generation;
- once reliable simulation performance is established studies on Diffraction Radiation and Smith Purcell radiation can be performed + moving on to the THz frequency region.
- complex models taking into account beam properties and surrounding hardware can be considered (Smith Purcell radiation, radiation from a capillary with periodic internal structure).

