Particle-In-Cell Based Beam Dynamics Simulations

Thomas Lau, E. Gjonaj and T. Weiland

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Technische Universität Darmstadt, Fachbereich Elektrotechnik und Informationstechnik
Schloßgartenstr. 8 , 64289 Darmstadt, Germany - URL: www.TEMF.de

Overview

- Motivation
- Finite Integration Technique
  - Non Conformal
  - Conformal
- Noise Reduction
  - Splitting Scheme
  - Dissipative Scheme
- Analytical Benchmark
- Simulations
- Conclusions

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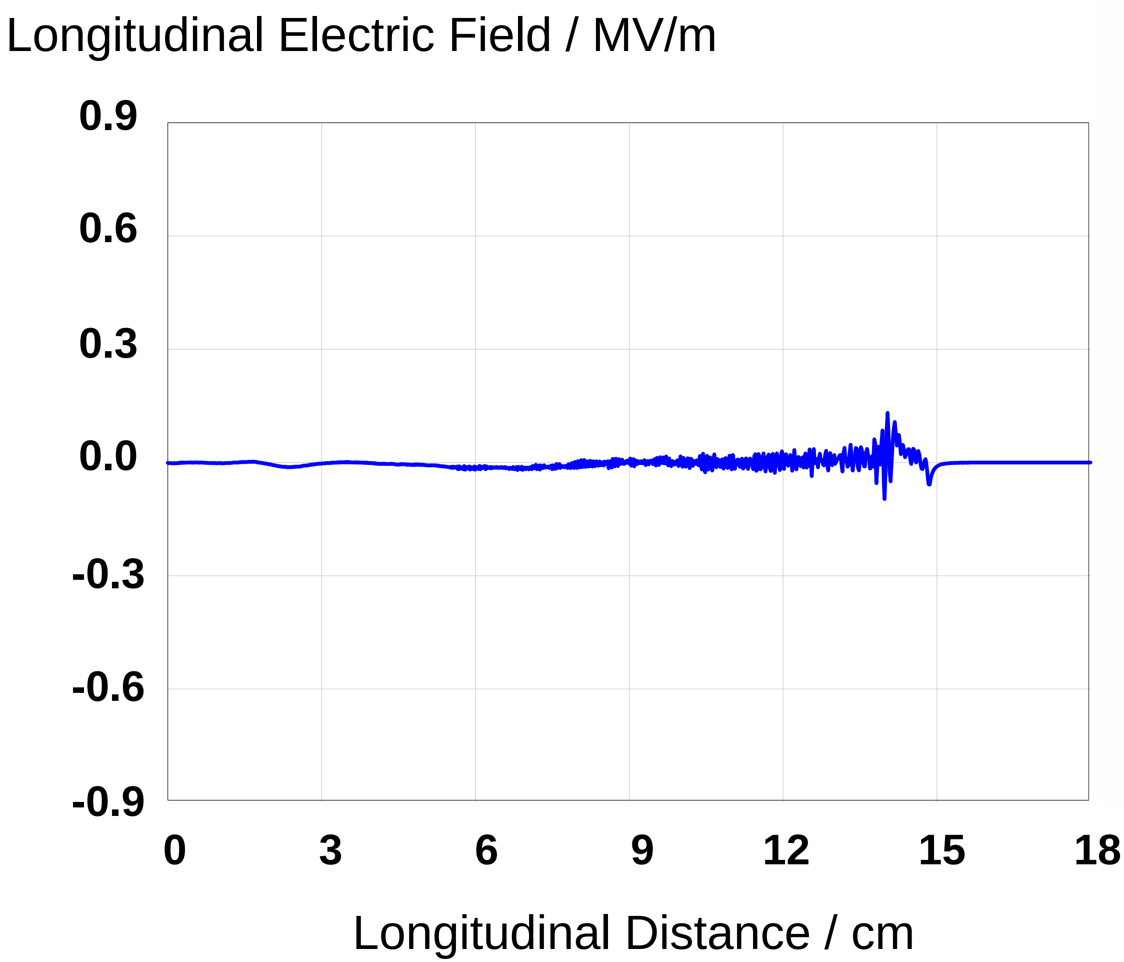
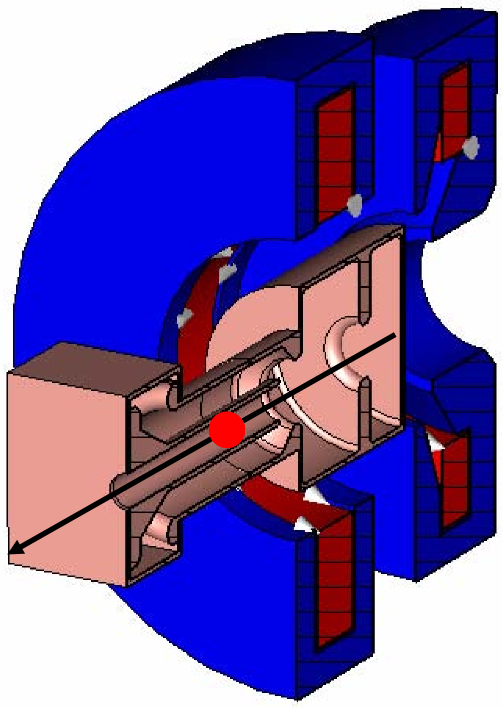
Motivation

- Simulation of relativistic electron beams
- Bunch is much smaller than the geometry





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Maxwell-Grid-Equations (Weiland, 1977)

Integral Maxwell Equations:

$$\oint_{\partial A} \vec{E} \cdot d\vec{s} = -\frac{\partial}{\partial t} \iint_A \vec{B} \cdot d\vec{A}$$

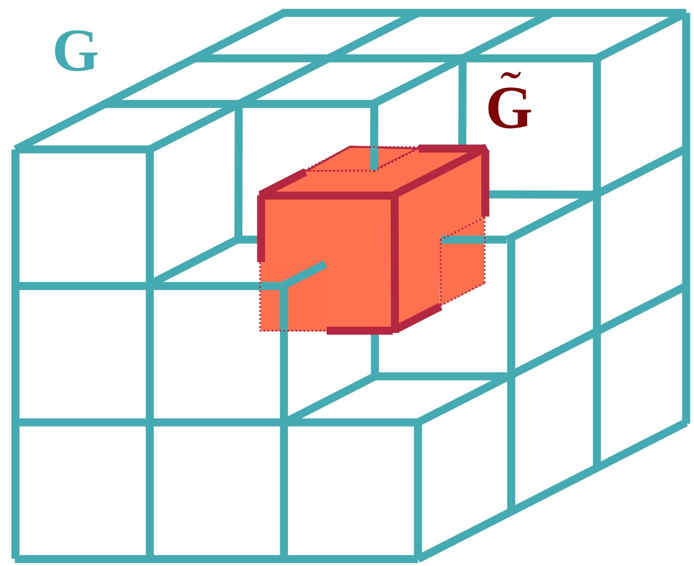
$$\oint_{\partial A} \vec{H} \cdot d\vec{s} = \iint_A \left(\frac{\partial}{\partial t} \vec{D} + \vec{J} \right) \cdot d\vec{A}$$

$$\oiint_{\partial V} \vec{B} \cdot d\vec{A} = 0$$

$$\oiint_{\partial V} \vec{D} \cdot d\vec{A} = \iiint_V \rho \, dV$$

Description by finite field *fluxes* and *voltages*

Grid-Dual-Grid Discretization:



$\mathbf{G} \rightarrow$ Primary grid

$\tilde{\mathbf{G}} \rightarrow$ Dual (orthogonal) grid

Maxwell-Grid-Equations (Weiland, 1977)

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$$\oiint_{\partial V} \vec{D} \cdot d\vec{A} = \iiint_V \rho \, dV$$

$$\oiint_{\partial V} \vec{B} \cdot d\vec{A} = 0$$

FIT

FIT Equations:

$$\mathbf{C}\widehat{\mathbf{e}} = -\frac{d}{dt}\widehat{\widehat{\mathbf{b}}}$$

$$\tilde{\mathbf{C}}\widehat{\mathbf{h}} = \frac{d}{dt}\widehat{\widehat{\mathbf{d}}} + \widehat{\widehat{\mathbf{j}}}$$

$$\tilde{\mathbf{S}}\widehat{\widehat{\mathbf{d}}} = \mathbf{q}$$

$$\mathbf{S}\widehat{\widehat{\mathbf{b}}} = 0$$

- <u>Exact</u> mapping in grid-space
- Material equations needed: $\widehat{\widehat{\mathbf{d}}} \to \widehat{\mathbf{e}}, \widehat{\widehat{\mathbf{b}}} \to \widehat{\mathbf{h}}$

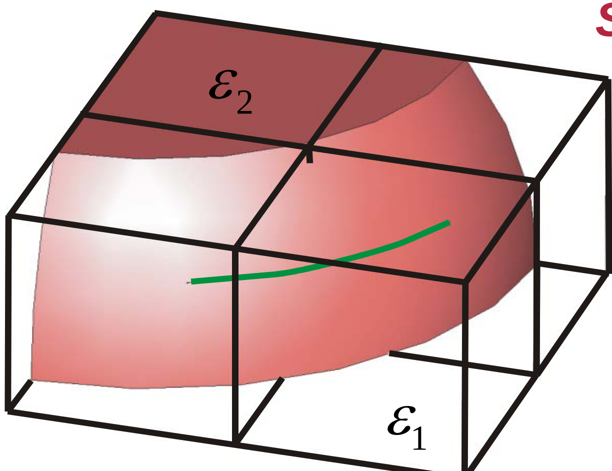
Material Operators. Staircase FIT

- Linear material operators
- Constructed by discretization
- Approximation depends on material operators only

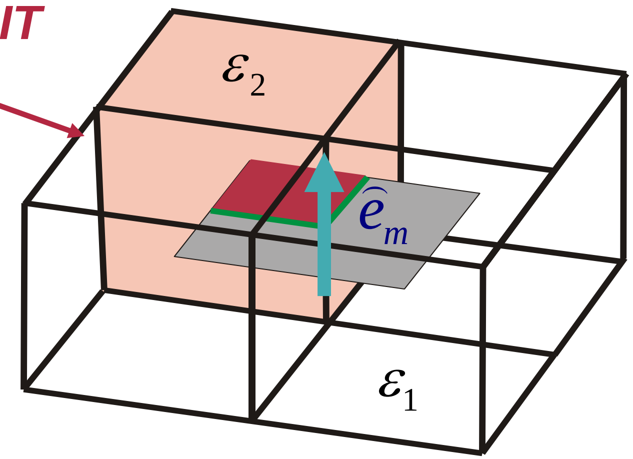
$$\vec{D} = \varepsilon \vec{E} \quad \Leftrightarrow \quad \widehat{\widehat{\mathbf{d}}} = \mathbf{M}_{\varepsilon} \widehat{\mathbf{e}}$$

$$\mu \vec{H} = \vec{B} + \vec{M} \quad \Leftrightarrow \quad \widehat{\mathbf{h}} = \mathbf{M}_{\mu^{-1}} \widehat{\widehat{\mathbf{b}}} + \widehat{\mathbf{M}}$$

$$\vec{J} = \sigma \vec{E} + \vec{J}_s \quad \Leftrightarrow \quad \widehat{\widehat{\mathbf{j}}} = \mathbf{M}_{\sigma} \widehat{\mathbf{e}} + \widehat{\widehat{\mathbf{j}}}_s$$



Staircaseing FIT



$\{\mathbf{M}_{\varepsilon}\}_{mm}$

- Diagonal, positive matrices for Cartesian grids

$$\widehat{\widehat{d}}_m \approx \left(\int_{A_m} \varepsilon \, dA \Big/ \int_{L_m} ds \right) \widehat{e}_m$$

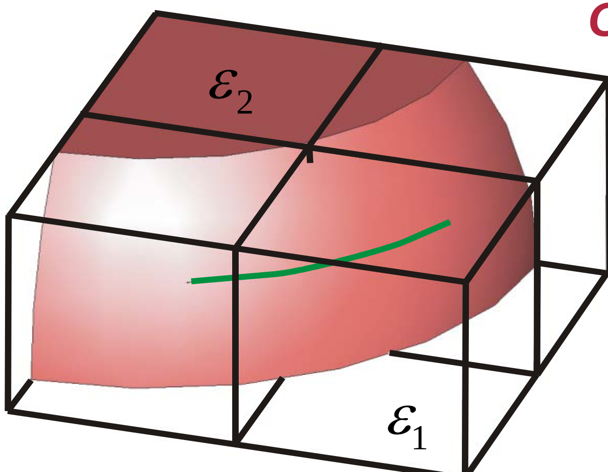
Material Operators. Conformal FIT

- Linear material operators
- Constructed by discretization
- Approximation depends on material operators only

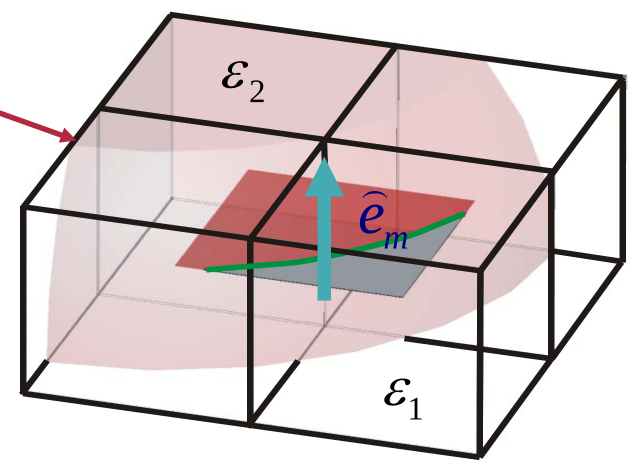
$$\vec{D} = \varepsilon \vec{E} \quad \Leftrightarrow \quad \widehat{\widehat{\mathbf{d}}} = \mathbf{M}_{\varepsilon} \widehat{\mathbf{e}}$$

$$\vec{H} = \mu \vec{B} \quad \Leftrightarrow \quad \widehat{\mathbf{h}} = \mathbf{M}_{\mu} \widehat{\widehat{\mathbf{b}}}$$

$$\vec{J} = \sigma \vec{E} + \vec{J}_s \quad \Leftrightarrow \quad \widehat{\widehat{\mathbf{j}}} = \mathbf{M}_{\sigma} \widehat{\mathbf{e}} + \widehat{\widehat{\mathbf{j}}}_s$$



Conformal FIT



$\{\mathbf{M}_{\varepsilon}\}_{mm}$

- Diagonal, positive matrices for Cartesian grids

$$\widehat{\widehat{d}}_m \approx \left(\int_{\tilde{A}_m} \varepsilon \, dA \Big/ \int_{L_m} ds \right) \widehat{e}_m$$

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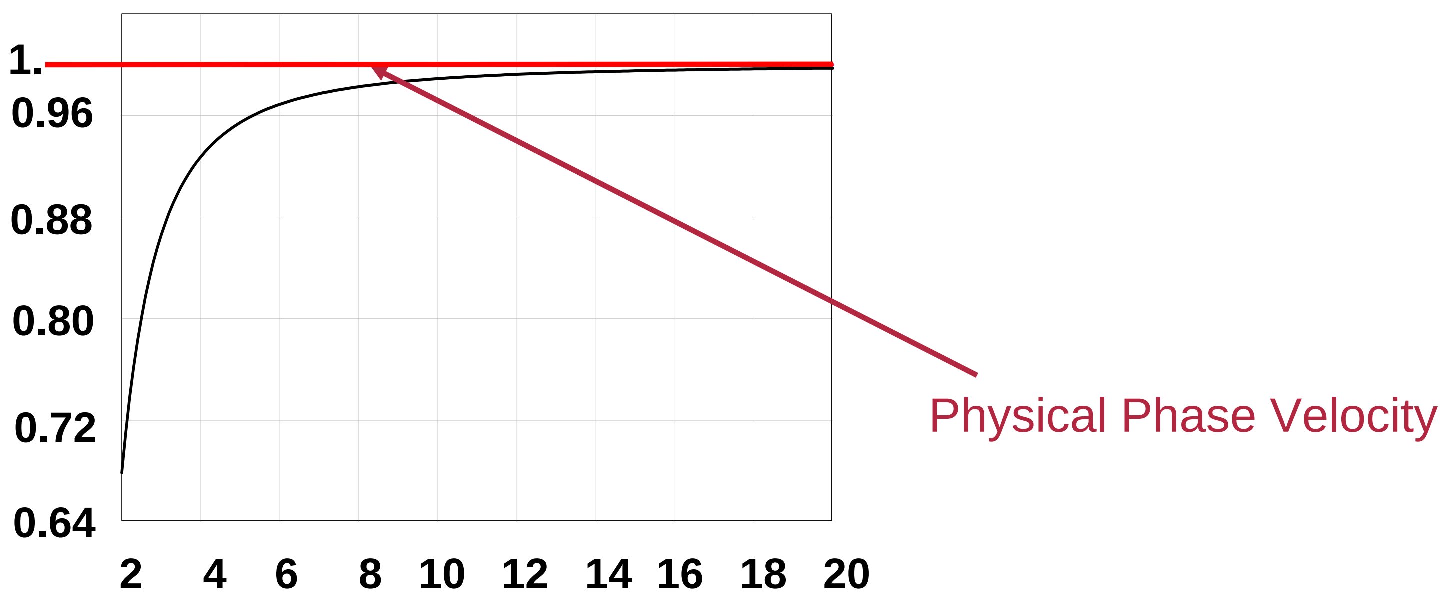
Leap-Frog Scheme

$$\begin{pmatrix} \widehat{\mathbf{h}}^{(n+1)} \\ \widehat{\mathbf{e}}^{(n+3/2)} \end{pmatrix} = \begin{pmatrix} \mathbf{1} & -\Delta t \cdot \mathbf{M}_{\mu^{-1}} \mathbf{C} \\ \Delta t \cdot \mathbf{M}_{\varepsilon^{-1}} \tilde{\mathbf{C}} & \mathbf{1} + \Delta t^2 \mathbf{M}_{\varepsilon^{-1}} \tilde{\mathbf{C}} \mathbf{M}_{\mu^{-1}} \mathbf{C} \end{pmatrix} \begin{pmatrix} \widehat{\mathbf{h}}^{(n)} \\ \widehat{\mathbf{e}}^{(n+1/2)} \end{pmatrix} + \Delta t \begin{pmatrix} 0 \\ \mathbf{M}_{\varepsilon^{-1}} \widehat{\mathbf{j}}_S^{(n+1)} \end{pmatrix}$$

Discrete Phase Velocity



Grid Points / Wave Length

Transversal Current Adjustment (TCA)

- Introduces an artificial damping of short wavelengths
- Formulation as Curl Curl operator ensures that neither new electric nor new magnetic charges are created by the artificial damping term

Artificial Damping Term

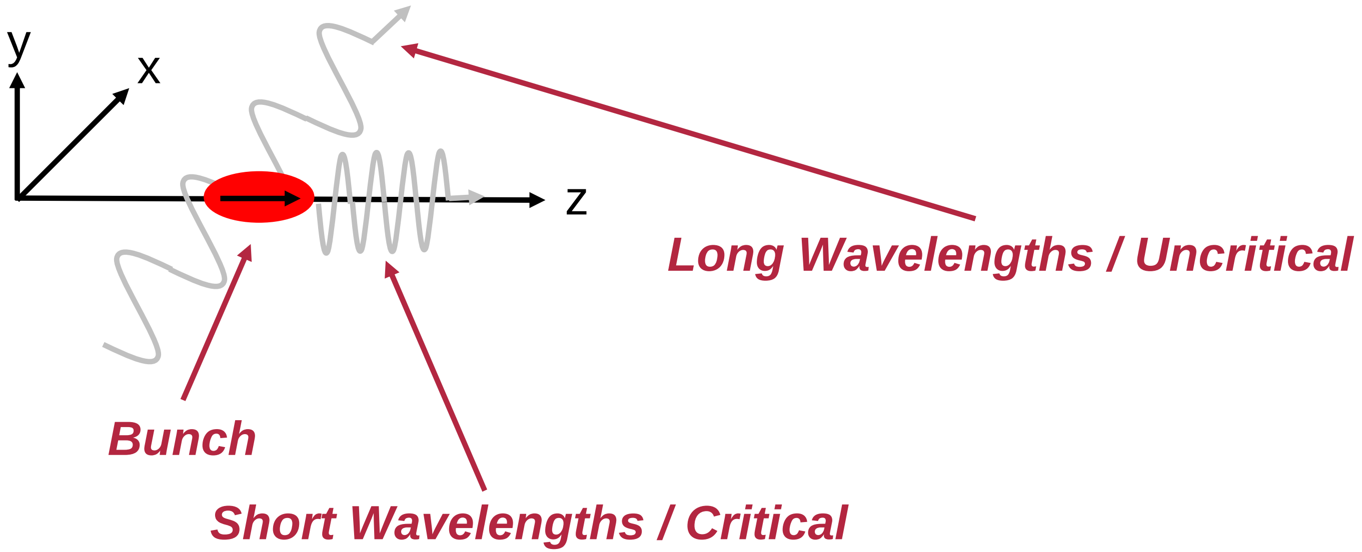
$$\begin{pmatrix} \widehat{\mathbf{h}}^{(n+1)} \\ \widehat{\mathbf{e}}^{(n+3/2)} \end{pmatrix} = \begin{pmatrix} \mathbf{1} + \alpha \Delta t^2 \mathbf{M}_{\varepsilon^{-1}} \tilde{\mathbf{C}} \mathbf{M}_{\mu^{-1}} \mathbf{C} & -\Delta t \cdot \mathbf{M}_{\mu^{-1}} \mathbf{C} \\ \Delta t \cdot \mathbf{M}_{\varepsilon^{-1}} \tilde{\mathbf{C}} & \mathbf{1} + \Delta t^2 \mathbf{M}_{\varepsilon^{-1}} \tilde{\mathbf{C}} \mathbf{M}_{\mu^{-1}} \mathbf{C} \end{pmatrix} \begin{pmatrix} \widehat{\mathbf{h}}^{(n)} \\ \widehat{\mathbf{e}}^{(n+1/2)} \end{pmatrix}$$

$$+\Delta t \begin{pmatrix} 0 \\ \mathbf{M}_{\varepsilon^{-1}} \widehat{\mathbf{j}}_s^{(n+1)} \end{pmatrix}$$

Transversal Current Adjustment (TCA)

- Easy to implement
- Has a variable damping parameter
  - The optimal value is problem dependent
- Decreases the stability limit of the Leap-Frog method
  - The time step has to be reduced
- There is minimal numerical overhead compared to the Leap-Frog method

Longitudinal Transversal Operator Splitting



Split the Maxwell equations, with respect to space, into a transversal and a longitudinal part

Noise Reduction

Longitudinal-Transversal Strang Splitting

$$\begin{pmatrix} \widehat{\mathbf{h}}^{(*)} \\ \widehat{\mathbf{e}}^{(*)} \end{pmatrix} = \begin{pmatrix} \mathbf{1} & -\frac{\Delta t}{2} \cdot \mathbf{M}_{\mu^{-1}} \mathbf{C}_T \\ \frac{\Delta t}{2} \cdot \mathbf{M}_{\varepsilon^{-1}} \tilde{\mathbf{C}}_T & \mathbf{1} \end{pmatrix} \begin{pmatrix} \widehat{\mathbf{h}}^{(n)} \\ \widehat{\mathbf{e}}^{(n+1/2)} \end{pmatrix} + \frac{\Delta t}{2} \begin{pmatrix} 0 \\ \mathbf{M}_{\varepsilon^{-1}} \widehat{\mathbf{j}}_S^{(n+1)} \end{pmatrix}$$

Transversal Update First Half Step

$$\begin{pmatrix} \widehat{\mathbf{h}}^{(**)} \\ \widehat{\mathbf{e}}^{(**)} \end{pmatrix} = \begin{pmatrix} \mathbf{1} & -\Delta t \cdot \mathbf{M}_{\mu^{-1}} \mathbf{C}_L \\ \Delta t \cdot \mathbf{M}_{\varepsilon^{-1}} \tilde{\mathbf{C}}_L & \mathbf{1} \end{pmatrix} \begin{pmatrix} \widehat{\mathbf{h}}^{(*)} \\ \widehat{\mathbf{e}}^{(*)} \end{pmatrix}$$

Longitudinal Update

$$\begin{pmatrix} \widehat{\mathbf{h}}^{(n+1)} \\ \widehat{\mathbf{e}}^{(n+3/2)} \end{pmatrix} = \begin{pmatrix} \mathbf{1} & -\frac{\Delta t}{2} \cdot \mathbf{M}_{\mu^{-1}} \mathbf{C}_T \\ \frac{\Delta t}{2} \cdot \mathbf{M}_{\varepsilon^{-1}} \tilde{\mathbf{C}}_T & \mathbf{1} \end{pmatrix} \begin{pmatrix} \widehat{\mathbf{h}}^{(**)} \\ \widehat{\mathbf{e}}^{(**)} \end{pmatrix} + \frac{\Delta t}{2} \begin{pmatrix} 0 \\ \mathbf{M}_{\varepsilon^{-1}} \widehat{\mathbf{j}}_S^{(n+1)} \end{pmatrix}$$

Transversal Update Second Half Step

Longitudinal-Transversal Strang Splitting

- Uses the largest time step possible for relativistic beams, the Courant time step
- Is 2 times more expensive than the Leap-Frog method, but the time step is 1.7 times greater
- Has zero dispersion along the beam axis at the Courant time step
- Is still second order accurate in space and time
- The splitting error creates magnetical and electrical charges
    - This seems not to be a problem in practical calculations

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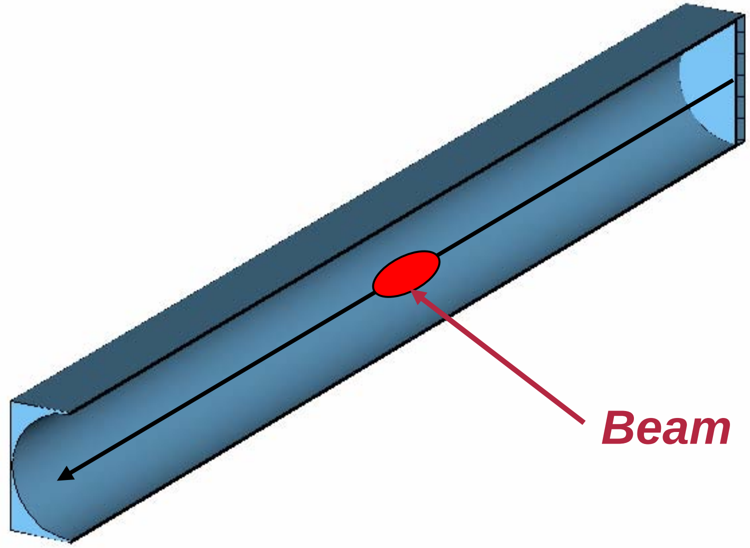
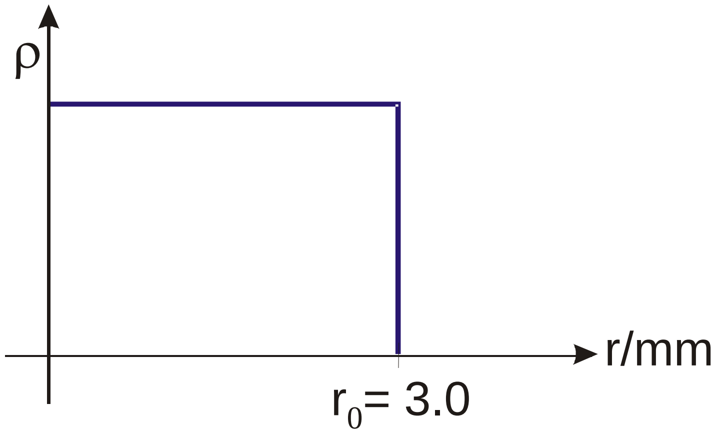
Analytical Benchmark

Bunch Parameters:

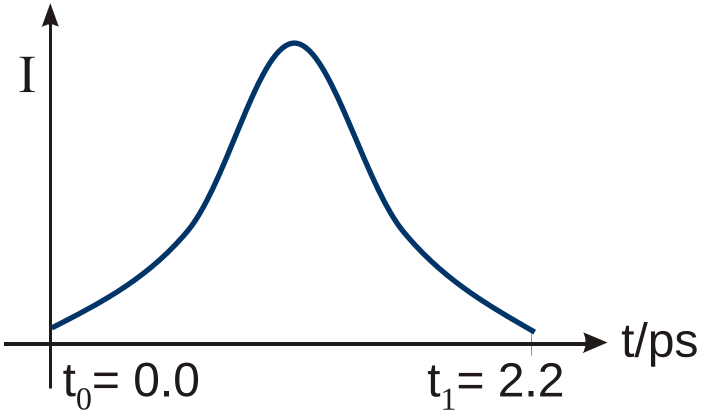
Q_{Bunch}	-1 / nC
β_{Bunch}	0.9
r_{Bunch}	3.0 / mm
l_{Bunch}	6.0 / mm
r_{Tube}	20.0 / mm



Radial Distribution:

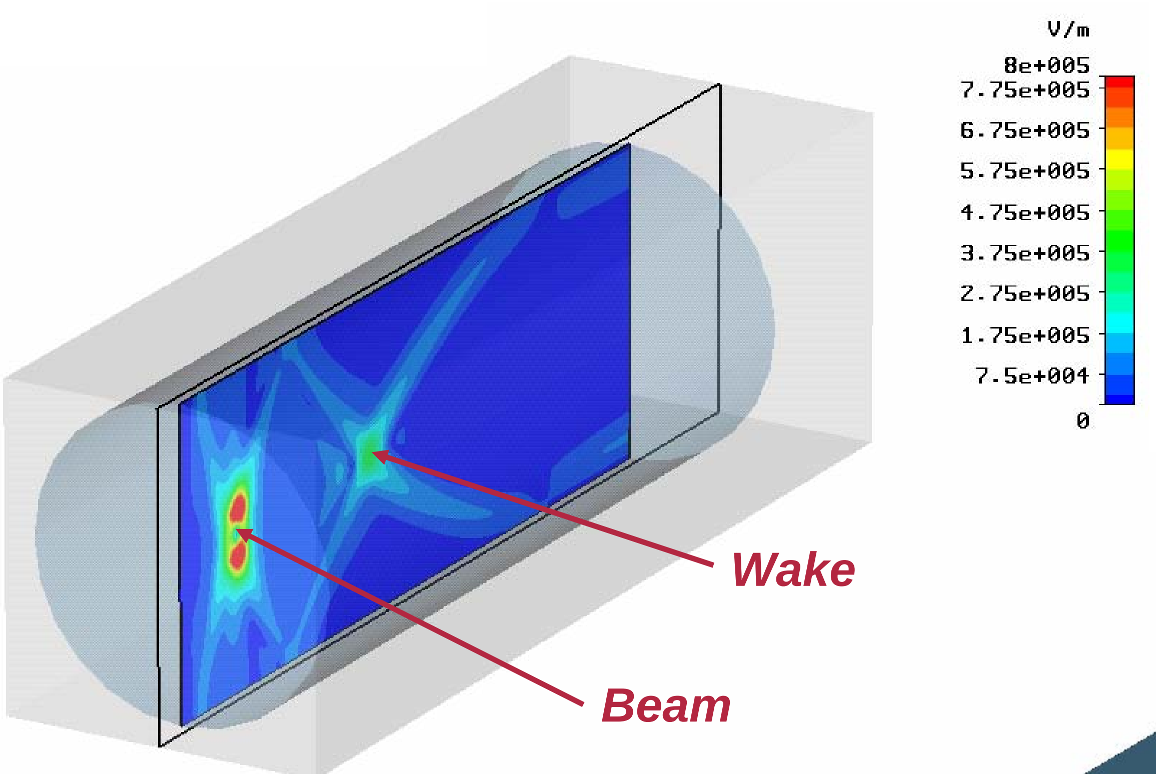


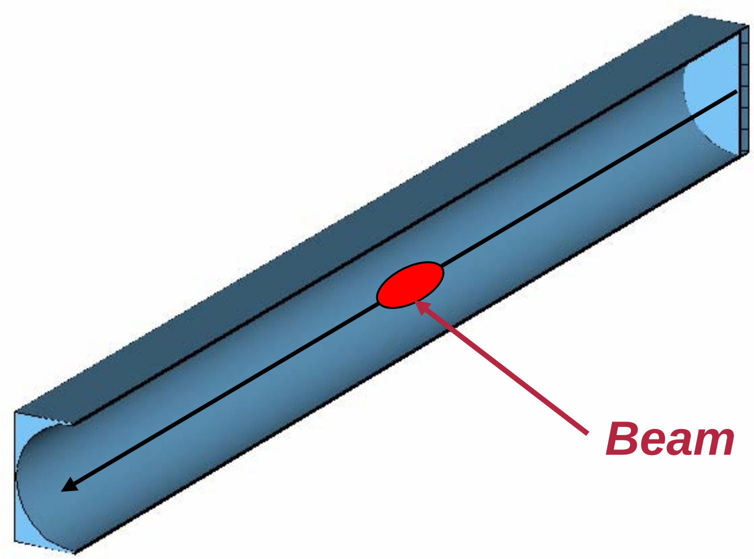
Gaussian Time Distribution:



Analytical Benchmark

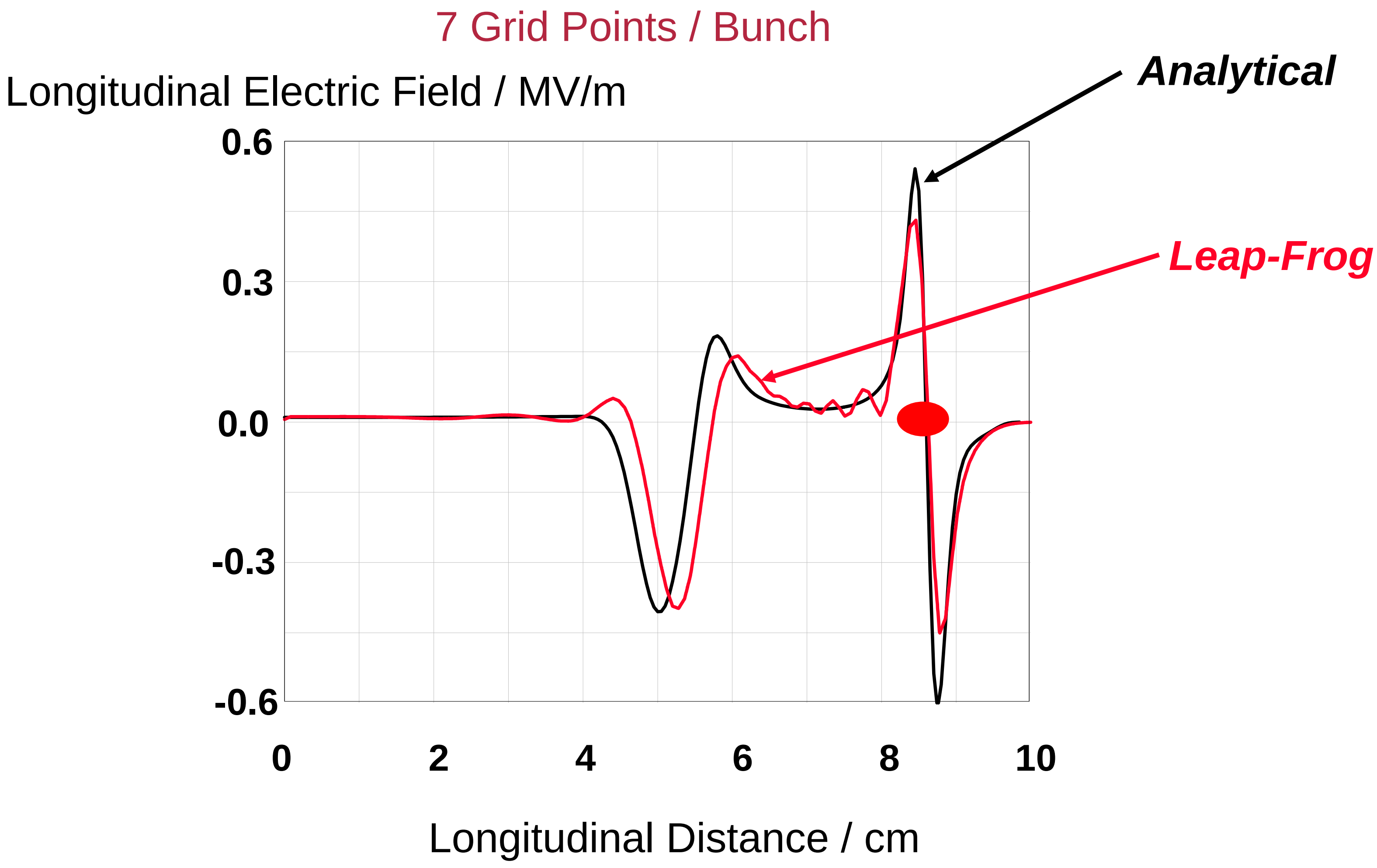
Absolute Value of Electrical Field in the Waveguide





Analytical Benchmark

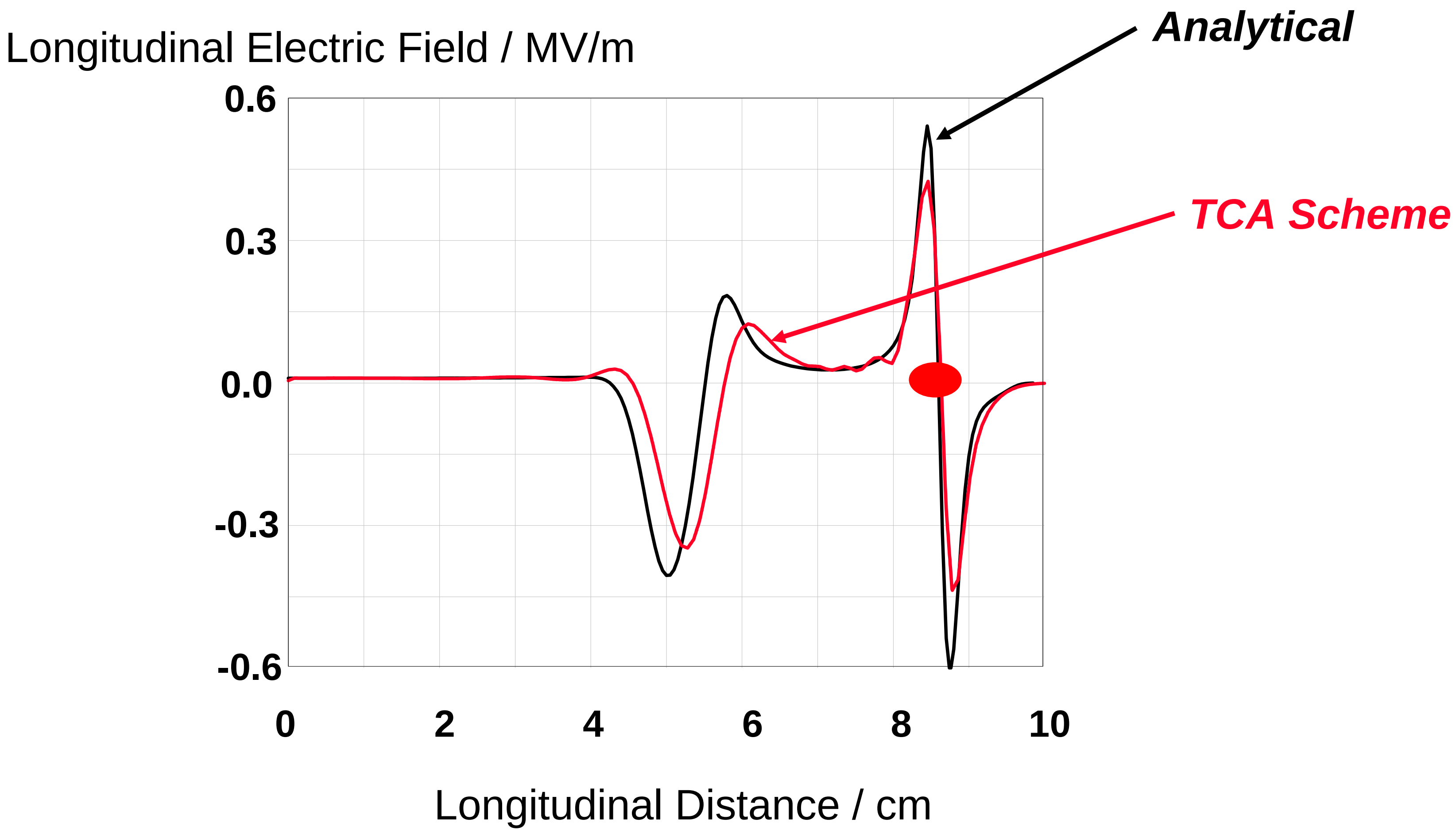
Longitudinal Electric Field on the Beam Axis



Analytical Benchmark

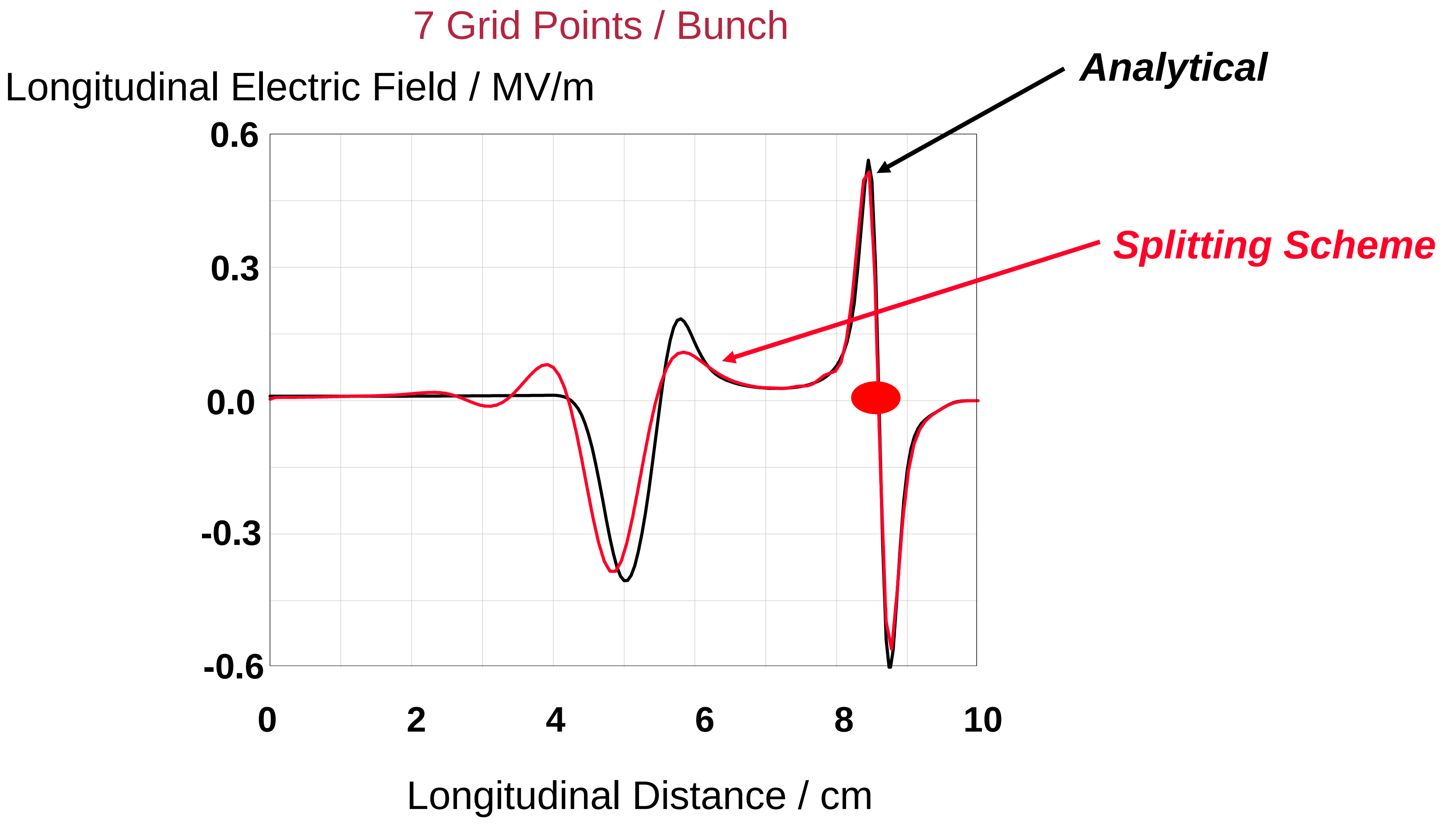
Longitudinal Electric Field on the Beam Axis

7 Grid Points / Bunch



Analytical Benchmark

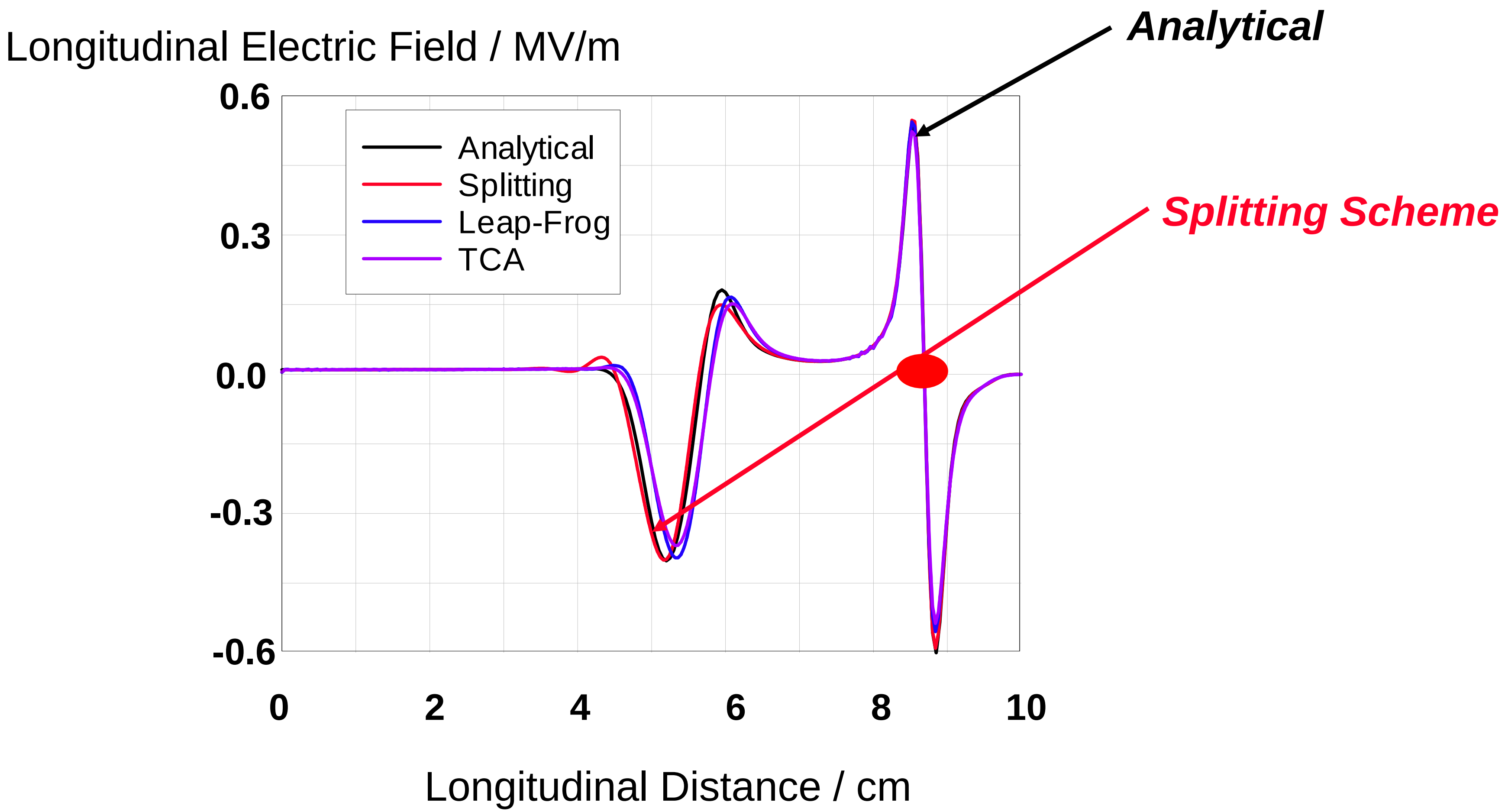
Longitudinal Electric Field on the Beam Axis



Analytical Benchmark

Longitudinal Electric Field on the Beam Axis

14 Grid Points / Bunch



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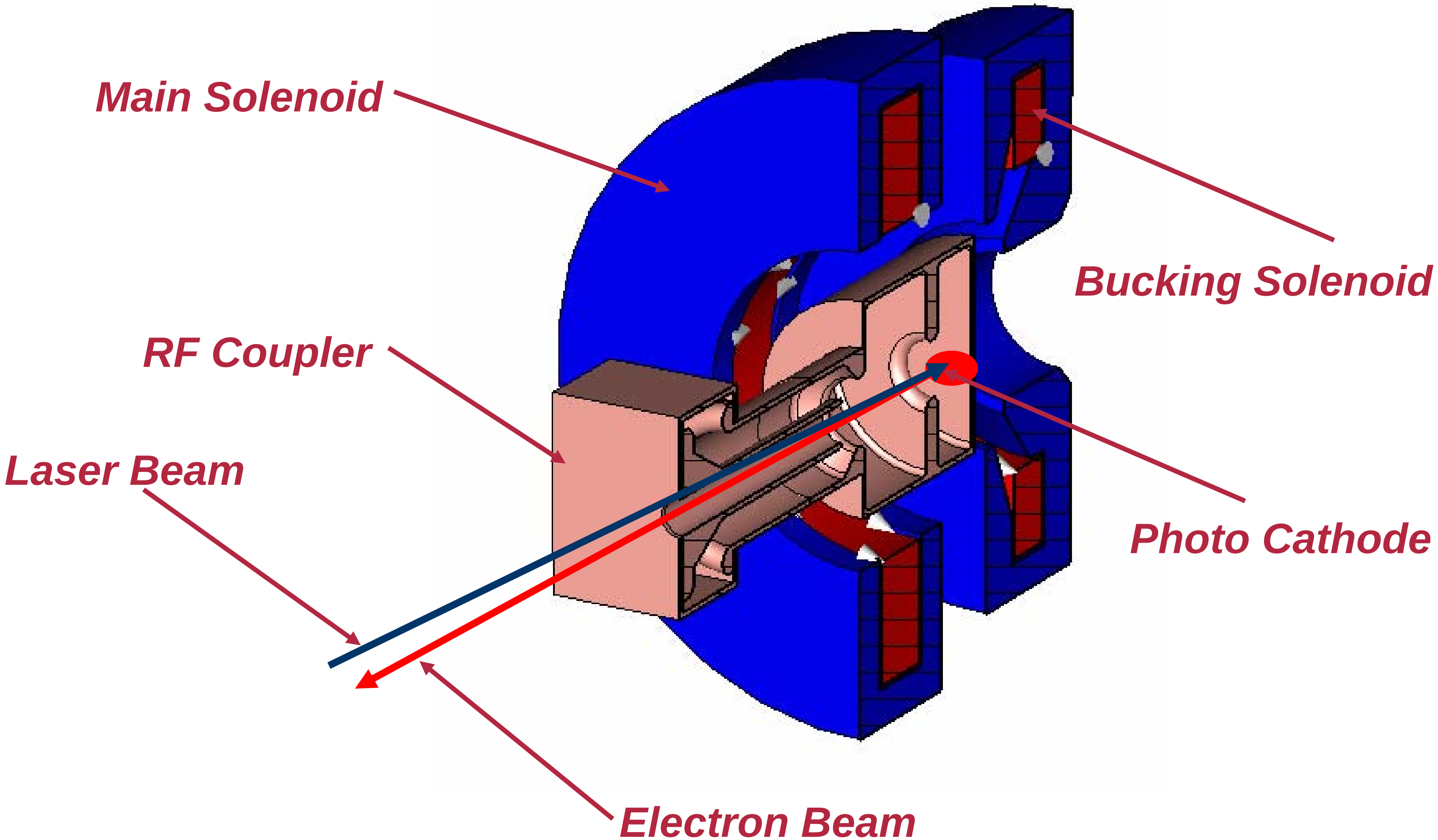
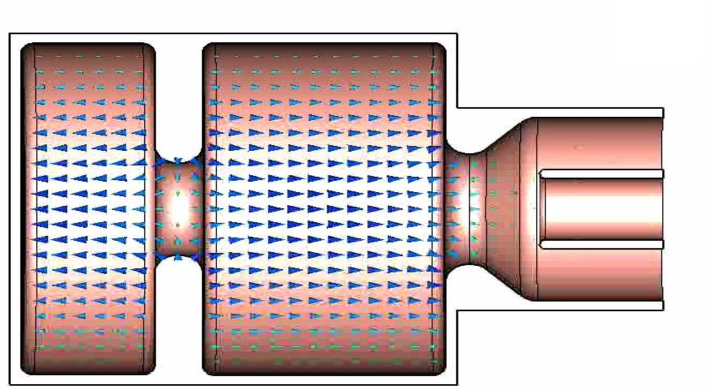
PITZ RF-Gun

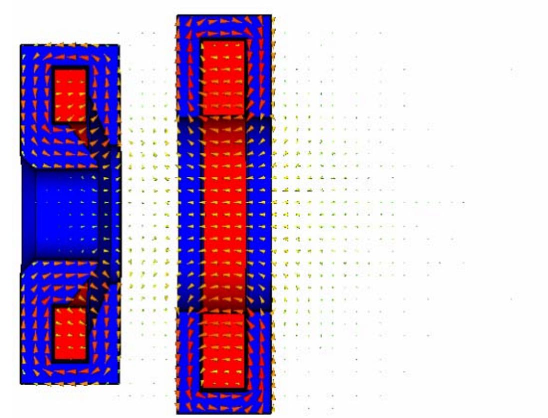

Main Solenoid
Bucking Solenoid
RF Coupler
Laser Beam
Photo Cathode
Electron Beam

Simulations

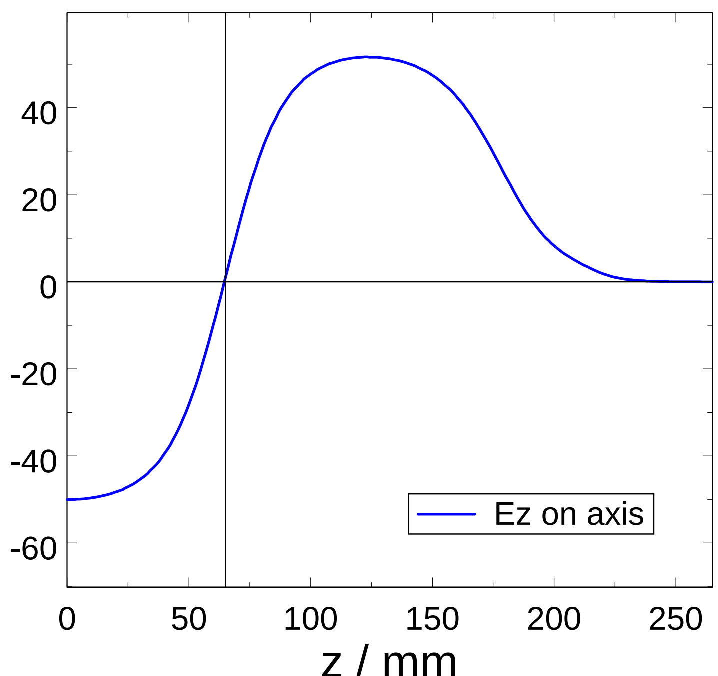
Cavity:



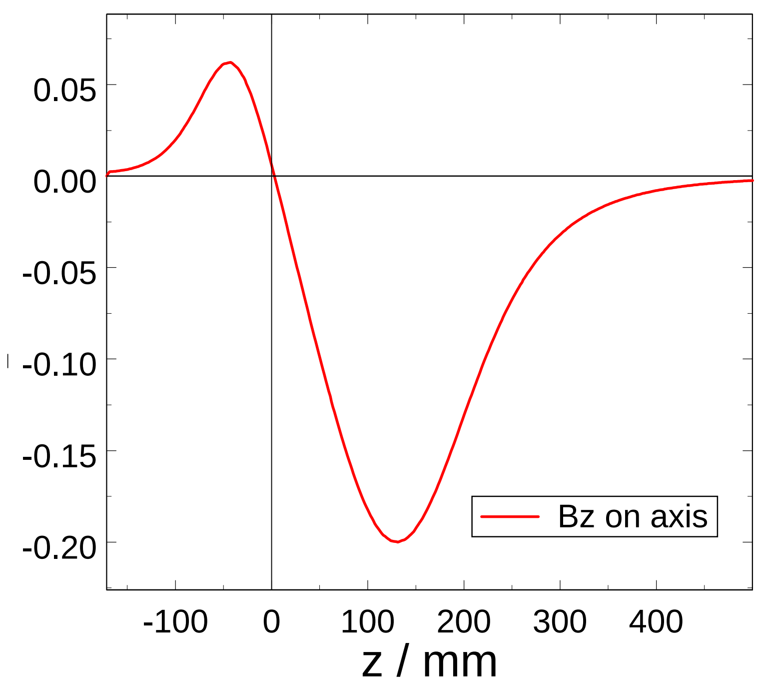
Solenoids:



Longitudinal Electric Field / MV/m



Longitudinal Magnetic Field / Tesla



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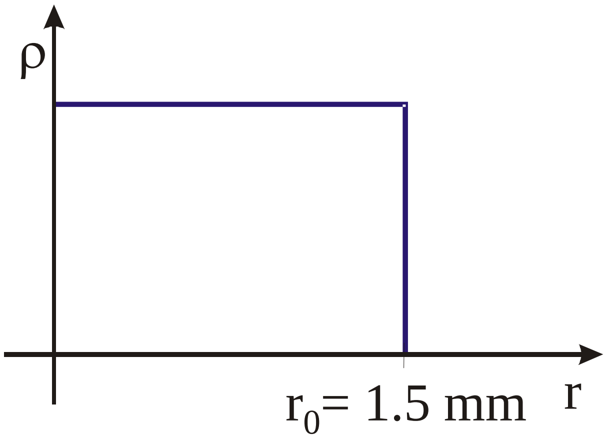
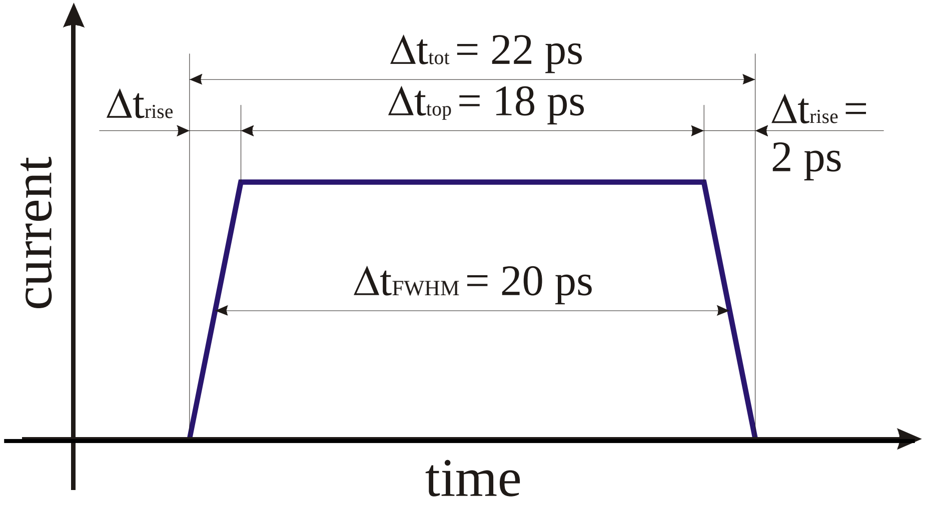
Bunch Parameters:

bunch radius	r_0 = 1.5 mm
bunch charge	q = -1 nC
bunch length	Δt_{FWHM} = 20 ps
rise/fall time	Δt_{rise} = 2 ps
reference phase	φ_0 = -47.4°
field at cathode	E_{cath} = -40.0 MV/m





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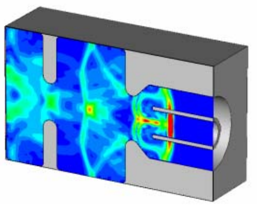
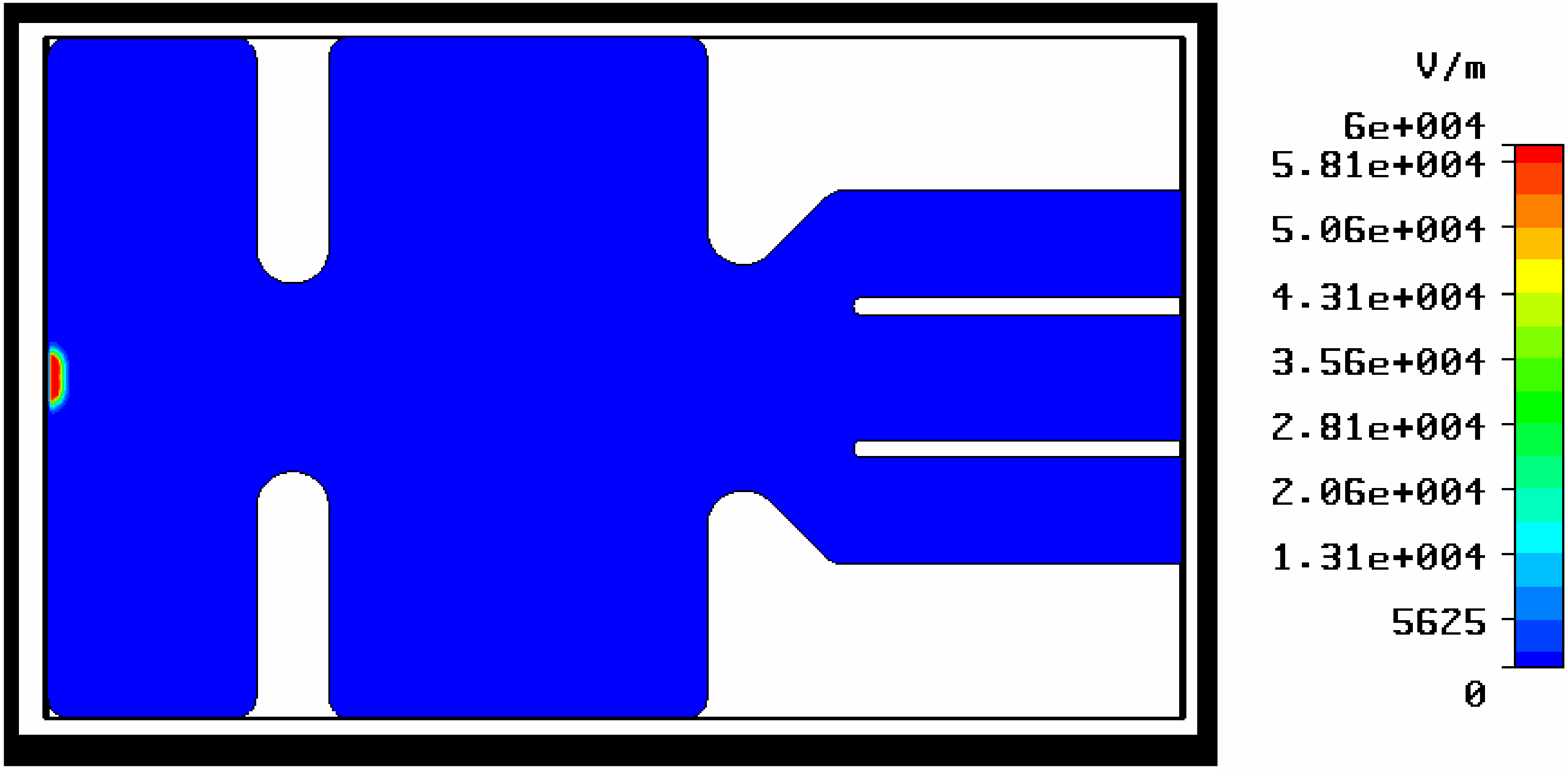
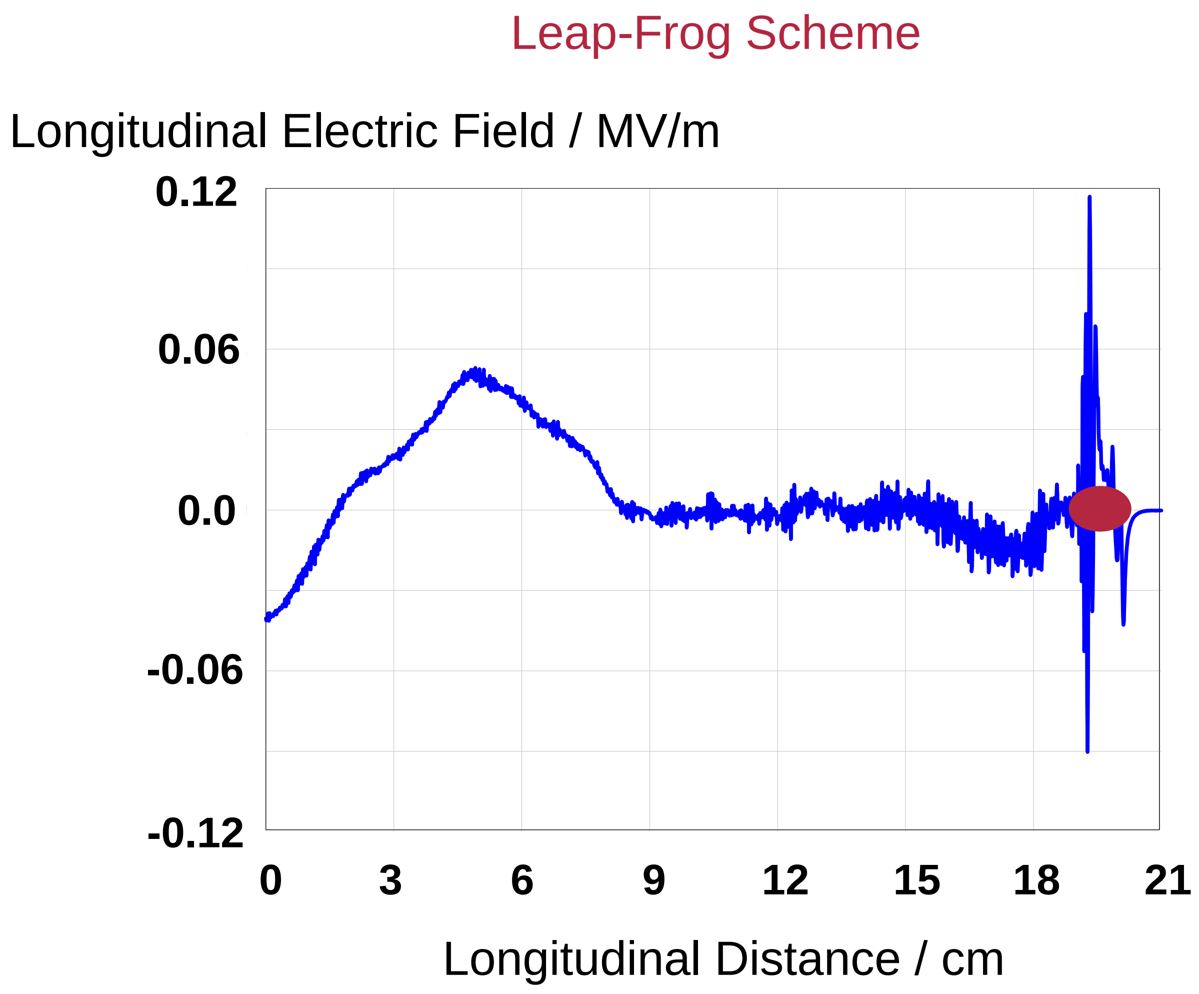
Electrical Space Charge Field in the PITZ - Cavity

- RF fields are precalculated
- Fully 3D simulation



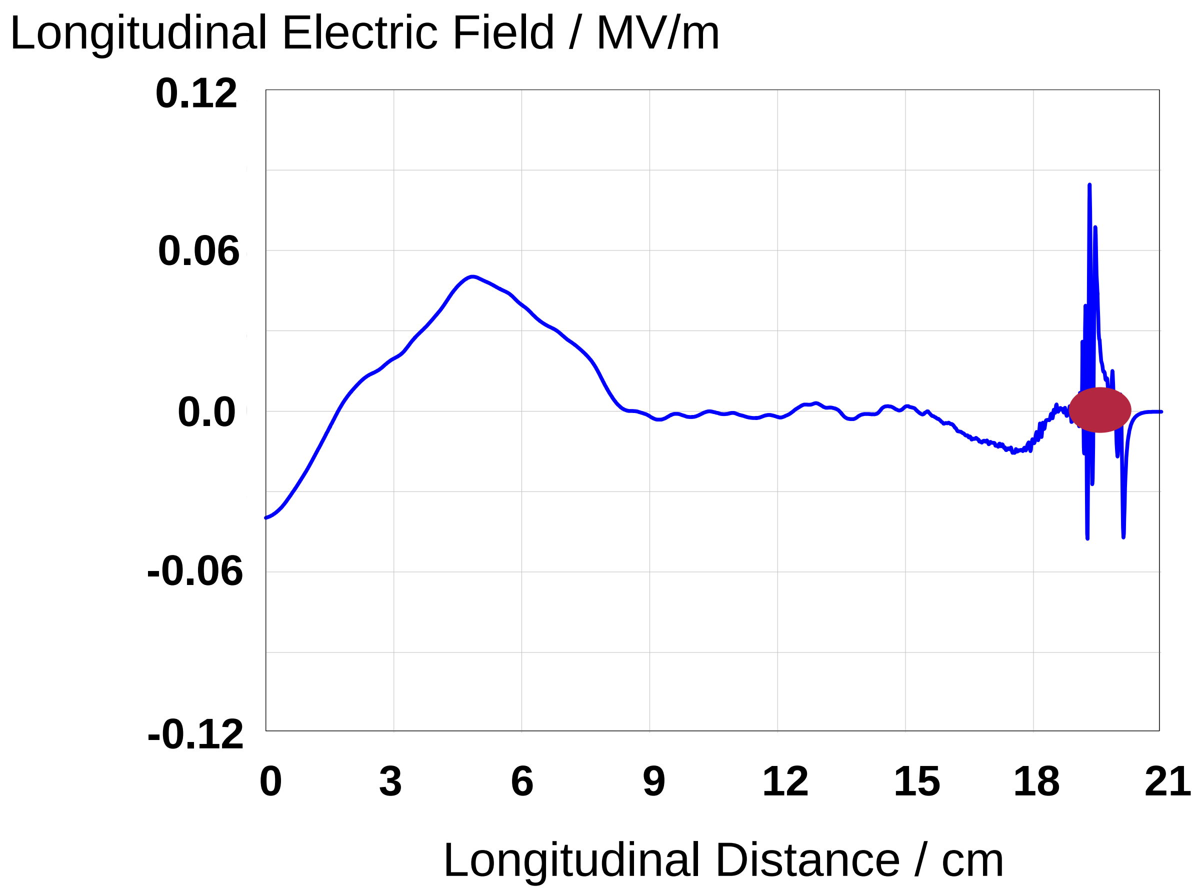


Longitudinal Electrical Field on the Beam Axis



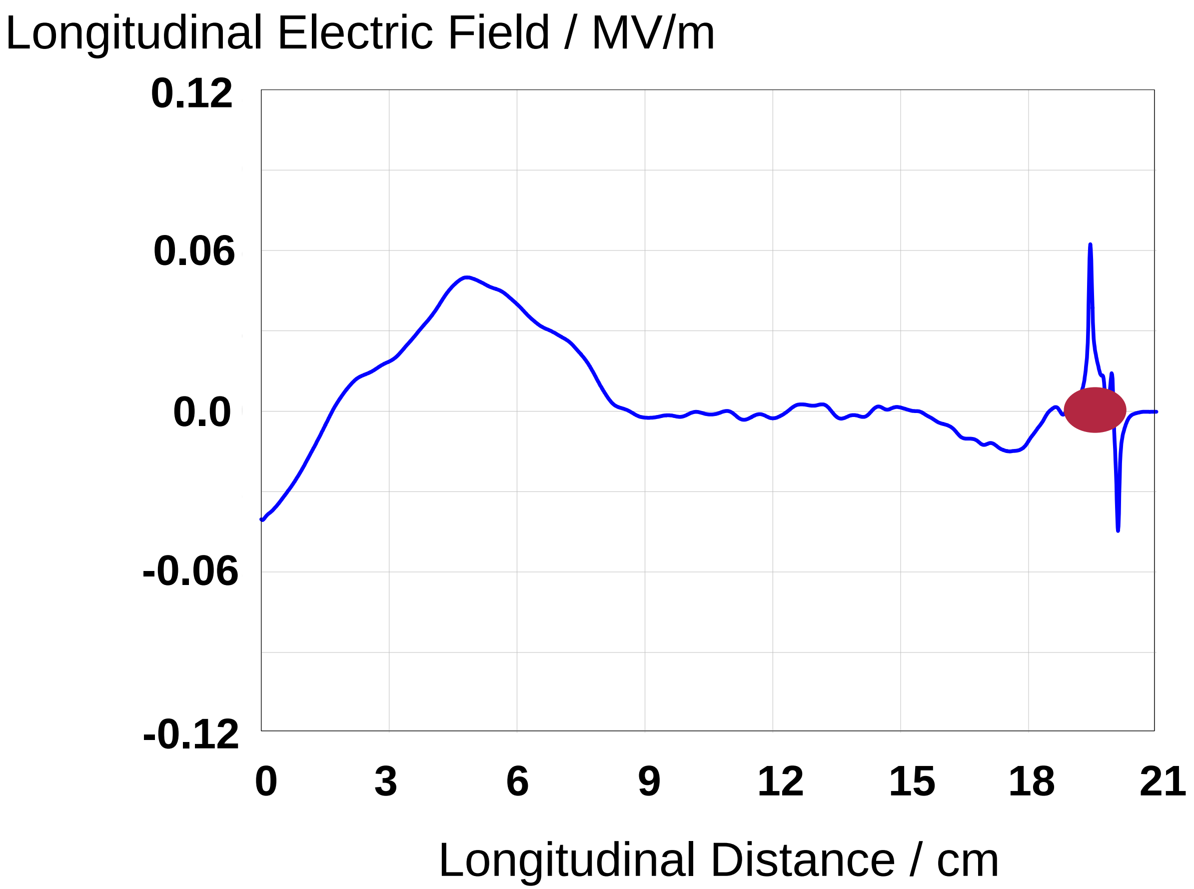
Longitudinal Electrical Field on the Beam Axis

TCA Scheme



Longitudinal Electrical Field on the Beam Axis

Splitting Scheme



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Conclusions

- The conventional method has a large numerical error
- Large structures with short bunches cannot be simulated.

S. Schnepp – Poster THPLT037 – „Investigation of Numerical Noise in PIC-codes“

S. Setzer – Poster WEPLT061 – „Influence of Beam Tube Obstacles on the Emittance of the PITZ Photoinjector“

E. Gjonaj – Poster THPLT035 – „Development of a 3D-Gun-Code based on a Charge Conserving Algorithm“

- Full 3D simulations of e.g.modern high brightness electron sources at in reach

Thank You for the Attention