



Methods and Simulation Tools for Cavity Design

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- Introduction
- Methods in Computational Electromagnetics (CEM)
- Examples of CEM Methods:
 - Finite Integration Technique (FIT)
 - Coupled S-Parameter Simulation (CSC)
- Simulation Tools
- Practical Examples
 - Some generalities
 - Some selected examples

Overview

Introduction

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Superconducting accelerator cavities



www.kek.jp/intra-e/press/2005/image/ilc1.jpg



[Podl], IAP Frankfurt/M.



http://www.linearcollider.org/newsline/images/2008/ 20080501_dc_1.jpg





... and some other types

Jefferson Lab / http://irfu.cea.fr/Images/astImg/2407_2.jpg http://www.physics.umd.edu/courses/Phys263/Kelly/cavity.jpg

=> Often chains of repeated structures, combined with flanges / coupling devices.

- I) Accelerating Mode:
- Do $v_{part}/(2f_{res})$ and L_{cell} match?
- How much energy does the particle gain?

$$\Delta E_{kin} = q_{part} \int_{z=0}^{z=L_{cav}} E_z(z) \cdot \cos(2\pi f_{res} z / v_{part} + \varphi_0) dz$$



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• How much energy is stored in the cavity?

$$W_{stored} = \frac{\mathcal{E}_0}{2} \iiint_{V_{cav}} \left| \vec{E}_{amplitude} \right|^2 dV = \frac{\mu_0}{2} \iiint_{V_{cav}} \left| \vec{H}_{amplitude} \right|^2 dV$$

• How big is the power loss in the wall? And how big is the unloaded quality factor?

$$P_{loss} = \frac{R_{surface}}{2} \oint_{cavity} \left| \vec{H}_{tan} \right|^2 dA = \frac{1}{2} \cdot \sqrt{\frac{\omega_{res}\mu}{2\sigma}} \oint_{cavity} \left| \vec{H}_{tan} \right|^2 dA; \quad Q_0 = \frac{\omega_{res}W_{stored}}{P_{loss}}$$

• Where are the maxima of electric (field emission) and magnetic (quench) field strength at the surface? Which values do they reach?

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II) Fundamental passband:

 All resonant frequencies! Which frequency spread does the fundamental passband have? How close is the next neighbouring mode to the accelerating mode? → Cell-to-Cell coupling → filling time

How strong is the beam interaction of all modes?
→ Look at "R over Q":

$$\frac{R}{Q} = \left(\frac{\Delta E_{kin}}{q_{part}}\right)^2 / \left(\omega_{res}W_{stored}\right)$$





III) Higher Order Modes (HOM):

- same questions as for fundamental passband
- wake potential \rightarrow kick factor
- special field profiles strongly confined far away

from couplers: "trapped modes"

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IV) Input and HOM-coupler/absorber:

- Q_{loaded} of all beam-relevant modes
- Field distortions due to coupler?
- Field distribution within the coupler
- V) Multipacting
- VI) Mechanical stability wrt. Lorentz Forces



- I) Accelerating mode
- **II)** Fundamental passband
- III) HOMs
- **IV) Input and HOM-coupler/absorber**
- V) Multipacting
- **VI)** Mechanical stability wrt. Lorentz Forces



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Eigenmodes provide most of the information needed:

100% of I) 100% of II) 80% of III) 25% of IV) 25% of V) 50% of VI)





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Most practical electrodynamics problems cannot be solved purely by means of analytical methods, see e.g.:

- radiation caused by a mobile phone near a human head
- shielding of an electronic circuit by a slotted metallic box
- mode computation in accelerator cavities, especially in chains of cavities

In many of such cases, numerical methods can be applied in an efficient way to come to a satisfactory solution.

Numerical Methods

Semi-analytical Methods

- Methods based on Integral Equations
- Method of Moments (MoM)

Discretization Methods

- Finite Difference Method (FD)
- Boundary Element Method (BEM)
- Finite Element Method (FEM)
- Finite Volume Method (FVM)
- Finite Integration Technique (FIT)

Possible Problems

- Need for geometrical simplifications \rightarrow MoM
- Violation of continuity conditions \rightarrow FD
- Unfavorable matrix structures \rightarrow BEM
- Unphysical solutions \rightarrow FEM if not mixed FEM
- Etc.

Discretization (I) of Solution itself

Discretization error; 1D and 2D



Picture source: http://www.integra.co.jp/eng/whitepapers/inspirer/inspirer.htm

Discretization (II) of Boundary of Solution Domain

In general: geometrical error





Structured "boundary-fitted" grid

Picture source:

http://www.sri.com/poulter/crash/crown_victoria/crvic_figures/fig_cvic2.html

Discretization (III) – Spatial Grid Types

Unstructured 2D grid:



Picture source: http://www.uni-karlsruhe.de/RZ/Dienste/GVM/DIENSTE/CAE-ANWENDUNGEN/ FIDAP/erfahrung/node46.html

Discretization (V) – Space and Time

space	\otimes	time	\rightarrow	grid space	×	grid time
\mathbb{R}^{3}	\otimes	${\mathbb R}^+$	\rightarrow	G	×	T



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Wave propagation in rectangular waveguide



Energy density of "wake fields" in the TESLA cavity





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FIT Discretization of Induction Law

 $\frac{\partial}{\partial t}\widehat{\hat{b}}_n$

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







 $\hat{e}_i + \hat{e}_j - \hat{e}_k - \hat{e}_l =$

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FIT Discretization of Gauss Law



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introduction of dual grid



FIT Discretization of Ampère's and Coulomb's Law

FIT equations on the dual grid



Maxwell's "Grid Equations" (MGE)

$$\operatorname{curl} \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\operatorname{curl} \mathbf{H} = -\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

$$\operatorname{div} \mathbf{D} = \rho$$

$$\operatorname{div} \mathbf{B} = 0$$

$$\mathbf{FIT}$$

$$\mathbf{D} = \varepsilon \mathbf{E}$$

$$\mathbf{B} = \mu \mathbf{H}$$

$$\mathbf{J} = \kappa \mathbf{E} + \mathbf{J}_{e}$$
T. Weiland, 1977, 1985
$$\mathbf{C} \,\widehat{\mathbf{e}} = -\frac{\partial}{\partial t} \,\widehat{\mathbf{b}}$$

$$\widetilde{\mathbf{C}} \,\widehat{\mathbf{h}} = -\frac{\partial}{\partial t} \,\widehat{\mathbf{d}} + \widehat{\mathbf{j}}$$

$$\widetilde{\mathbf{S}} \,\widehat{\mathbf{d}} = \mathbf{q}$$

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

$$\widehat{\mathbf{b}} = \mathbf{M}_{\varepsilon} \,\widehat{\mathbf{b}}$$

$$\widehat{\mathbf{b}} = \mathbf{M}_{\varepsilon} \,\widehat{\mathbf{b}}$$

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Shape Approximation on Cartesian Grids



U. van Rienen, H.-W. Glock

FIT on Triangular Grids

Grid

Dual grid



→ URMEL-T

U. van Rienen 1983



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FIT on Non-Orthogonal Grids



Field in model of 1 cell

<u>Hilgner</u>, <u>Schuhmann</u>, Weiland TU Darmstadt 1998



Maxwell's "Grid Equations" (MGE) → Curl Curl Equation

$$\operatorname{curl} \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\operatorname{curl} \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

$$\operatorname{div} \mathbf{D} = \rho$$

$$\operatorname{div} \mathbf{B} = 0$$

$$\mathbf{D} = \varepsilon \mathbf{E}$$

$$\mathbf{B} = \mu \mathbf{H}$$

$$\mathbf{J} = \kappa \mathbf{E} + \mathbf{J}_{e}$$
T. Weiland, 1977, 1985
$$\mathbf{C} \, \widehat{\mathbf{e}} = -\frac{\partial}{\partial t} \, \widehat{\mathbf{b}}$$

$$\widetilde{\mathbf{C}} \, \widehat{\mathbf{h}} = \frac{\partial}{\partial t} \, \widehat{\mathbf{d}} + \widehat{\mathbf{j}}$$

$$\widetilde{\mathbf{C}} \, \widehat{\mathbf{h}} = \frac{\partial}{\partial t} \, \widehat{\mathbf{d}} + \widehat{\mathbf{j}}$$

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$$\mathbf{C} \, \widehat{\mathbf{h}} = \frac{\partial}{\partial t} \, \widehat{\mathbf{d}} + \widehat{\mathbf{j}}$$

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

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

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

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

$$\mathbf{S} \, \widehat{\mathbf{b}} = \mathbf{M}$$

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Curl-Curl-Eigenvalue Equation

- $\widehat{\widehat{\boldsymbol{j}}}_{\mathcal{S}}\equiv\boldsymbol{0}$
- $\sigma = 0, \quad \varepsilon, \mu \text{ real} \quad (\text{loss-free})$

(no current excitation)

$$\mathbf{M}_{\varepsilon}^{-1}\,\,\tilde{\mathbf{C}}\mathbf{M}_{\mu^{-1}}^{-1}\mathbf{C}\,\,\widehat{\mathbf{e}}=\omega^{2}\widehat{\mathbf{e}}$$

eigenvalue problem

 $Ax = \lambda x$

$$\mathbf{A}_{\mathrm{CC}} = \mathbf{M}_{\varepsilon}^{-1} \; \tilde{\mathbf{C}} \mathbf{M}_{\mu-1} \mathbf{C}$$

$$\varepsilon^{-1}$$
 curl μ^{-1} curl $\mathbf{E} = \omega^2 \mathbf{E}$

Curl-Curl-Eigenvalue Equation

Use transformation $\hat{\mathbf{e}}' = \mathbf{M}_{\varepsilon}^{1/2} \hat{\mathbf{e}}$ to derive an equation with symmetric system matrix

$$\mathbf{M}_{\varepsilon}^{1/2}\widetilde{\mathbf{C}}\mathbf{M}_{\mu^{-1}}^{-1/2} \ \widetilde{\mathbf{C}}\mathbf{M}_{\varepsilon}^{-1/2} \ \widetilde{\mathbf{e}}^{\,\prime} = \omega^2 \ \widetilde{\mathbf{e}}^{\,\prime}$$

system matrix
$$\mathbf{A}' = \mathbf{M}_{\varepsilon}^{1/2} \mathbf{A}_{CC} \mathbf{M}_{\varepsilon}^{-1/2}$$

 $= \mathbf{M}_{\varepsilon}^{-1/2} \tilde{\mathbf{C}} \mathbf{M}_{\mu-1} \mathbf{C} \mathbf{M}_{\varepsilon}^{-1/2}$
 $= \left(\mathbf{M}_{\varepsilon}^{-1/2} \tilde{\mathbf{C}} \mathbf{M}_{\mu}^{-1/2}\right) \left(\mathbf{M}_{\varepsilon}^{-1/2} \tilde{\mathbf{C}} \mathbf{M}_{\mu}^{-1/2}\right)^{T}$ is symmetric

Solution Space of Eigenvalue Problem

system matrix
$$\mathbf{A}' = \mathbf{M}_{\varepsilon}^{1/2} \mathbf{A}_{CC} \mathbf{M}_{\varepsilon}^{-1/2}$$

 $= \mathbf{M}_{\varepsilon}^{-1/2} \tilde{\mathbf{C}} \mathbf{M}_{\mu-1} \mathbf{C} \mathbf{M}_{\varepsilon}^{-1/2}$
 $= \left(\mathbf{M}_{\varepsilon}^{-1/2} \tilde{\mathbf{C}} \mathbf{M}_{\mu}^{-1/2}\right) \left(\mathbf{M}_{\varepsilon}^{-1/2} \tilde{\mathbf{C}} \mathbf{M}_{\mu}^{-1/2}\right)^{T}$ is symmetric

Eigenvalues of A'

(and thus of \mathbf{A}_{CC} as well) are

1. real

2. non-negative

because

- **1. A**['] is symmetric
- **2.** $\mathbf{A}^{\cdot} = \text{matrix} \cdot (\text{matrix})^{\mathsf{T}}$

Eigenfrequencies ω_i are

real and non-negative

as it should be for a loss-less

resonator



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Coupled S-Parameter Calculation





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 $\textbf{CST MICROWAVE STUDIO} \mathbb{R}$

- -Transient Solver
- Eigenmode Solver
- Frequency Domain Solver
- Resonant: S-Parameters and Fields
- Integral Equations Solver

- Predecessors for eigenmode calculation: MAFIA, URMEL, URMEL-T



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• Tangential vector basis functions enabled the highly accurate finite element method for electromagnetic field solution

Technical Library

- Transfinite element method for fast and accurate multi-mode S-parameter extractions
- · Automatic mesh generation and adaptive refinement for reliable, repeatable and efficient results

http://www.ansoft.com/products/hf/hfss/

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ACE3P - Advanced Computational Electromagnetic Simulation Suite developed at SLAC by the group around Kwok Ko, Cho NG et al.

Module Name	Short Description	Home Institution
<u>Omega3P</u>	Frequency domain solver for computing resonant modes (with damping)	SLAC
[S3P]	Frequency domain solver for evaluating scattering parameters	SLAC
[T3P]	Time-domain solver for calculating transient effects and wakefields	SLAC
[Pic3P]	Particle-in-cell code for simulating space charge dominated devices	SLAC
[Track3P]	Particle tracking code for simulating multipacting and dark current	SLAC
[TEM3P]	Multi-physics module that includes electromagnetic, thermal and mechanical effects	SLAC
Paraview	Advanced visualization and analysis software	paraview.org

\rightarrow See examples in next part of the talk

https://confluence.slac.stanford.edu/display/AdvComp/Omega3P

ACE3P Suite



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Workflow of eigenmode computation



Passband Fields with $E_{tan} = 0$ in middle of the cavity

Make use of symmetry \rightarrow compute only $\frac{1}{2}$ of the cavity



Passband Fields with $H_{tan} = 0$ in middle of the cavity

Use of symmetry → compute only ½ of the cavity

Needs of course 2 (shorter) runs!

Visualization of full cavity provided by CST MWS

Even 1/8 part might be enough for computation





Passband Fields altogether





... which seems to obey some rule ?!

Computed with CST MWS

Passband fields altogether





fact:
$$f_{mode} \approx \frac{f_0 + f_{\pi}}{2} \left[1 - \frac{\kappa_{cc}}{2} \cos(\varphi) \right]$$

κ_{cc} : cell-to-cell coupling; compare K. Saito's talk

Computed with CST MWS

So, what are passbands?

Cavities built by chains of *identical cells* show resonances in certain frequency intervalls, called passbands, *determined only by the shape of the elementary cell*.

The distribution of resonances in the band depends on the number of cells in the chain:



Periodic Boundary Conditions

In fact, it is possible, to calculate the spectrum of an infinite chain by discretizing a single cell (exploiting other symmetries as well) ...:



... and to preset the cell-to-cell phase advance by application of an appropriate longitudinal boundary condition.

Computed with CST MWS

Periodic Boundary Conditions

This needs only one single run for each $\Delta\phi,$ but gives eigenmode frequencies of several passbands with a very small grid (here 19,000



What are Monopole-, Dipole-, Quadrupole-Modes?

Consider structures of axial circular symmetry. Then all fields belong to classes with invariance to certain azimuthal rotations:



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Trapped Mode Analysis

Search for strongly confined field distributions by simulating same structure with different waveguide terminations at beam pipe ends. Compare spectra! Small frequency shifts indicate weak coupling.



Computed with CST MWS



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Niobium; acceleration at 1.3 GHz





Computed with 2D-simulation of upper half; only azimuthal symmetry exploited MAFIA



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Higher Order Modes in TESLA Structure

Dipole mode 28, f = 2. 574621 GHz



Dipole mode 29, f = 2. 584735 GHz



CSC - 9-Cell Resonator with Couplers



• CSC: "Coupled S-Parameter Calculation" allows for combination of 2D- and 3D-simulations

K. Rothemund; H.-W. Glock; U. van Rienen. Eigenmode Calculation of Complex RF-Structures using S-Parameters. IEEE Transactions on Magnetics, Vol. 36, (2000): 1501-1503.

CSC - Resonator Chain – Variation of Tube Length



Weak dependence on position

Computed with MAFIA, CST MWS and our own Mathematica Code for CSC

Effect of Changed Coupler Design*

CSC to determine S-parameters of various object combinations

*New concept: M. Dohlus, DESY; ** Modal coeff. computed by M. Dohlus

H.-W. Glock, K. Rothemund

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Comparison: HOM(original) – HOM(mirrowed)

H.W. Glock; K. Rothemund; D. Hecht; U. van Rienen. S-Parameter-Based Computation in Complex Accelerator Structures: Q-Values and Field Orientation of Dipole Modes. Proc. ICAP 2002

Computational Needs for the European XFEL

ICAP 2009

Some of his slides ... Courtesy to Martin Dohlus

Martin Dohlus DESY, Hamburg

integrated transverse fields are orders of magnitude smaller than longitudinal field; max(Ez)~200

see W. Ackermann, Thursday afternoon

Courtesy of M. Dohlus, DESY – ICAP 2009

Higher Modes (HOM couplers and absorbers)

absorbers in interconnections between modules T > 70K

Courtesy of M. Dohlus, DESY – ICAP 2009

Higher Modes - HOM couplers

periodic rz simulation for one cell:

dispersion diagrams (monopole, dipole, ...) are usefull to localize bands of modes (multi-cell structures) \rightarrow rough estimate of *f* and *k* values

broad band xyz simulation of one cavity (closed beam pipes):

estimate of f, k and Q values \rightarrow investigation of multi bunch effects

T. Khabibouline, FERMILAB, see FERMILAB-TM2210, TESLA-FEL 2003-01

T. Khabibouline, FERMILAB, see FERMILAB-TM2210, TESLA-FEL 2003-01

models for cavity strings with geometric imperfections

still difficult: f.i. coupled S-matrix approach (TESLA module 3rd dipole band) or rz-caluclations (→ trapped modes, PEC environment)

Courtesy of M. Dohlus, DESY – ICAP 2009

Models for Mode Absorption (based on field calculation)

model with symmetry of revolution sufficient ? doable (if at all) only for rz-geometry

Models for Mode Absorption (geometrical optics)

cryoloss:

(Voss, Clemens, Dohlus)

real rz-surface geometry of module; ray tracing; plane wave loss model for surface reflections; intensity reduction of plane wave; summation of surface losses \rightarrow distribution of losses

Models for Mode Absorption (geometrical optics)

= infinite string of cold modules !

Courtesy of M. Dohlus, DESY – ICAP 2009

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Models for Mode Absorption (geometrical optics)

Courtesy of M. Dohlus, DESY – ICAP 2009

SLAC Parallel EM Codes

Simulation Multipacting and Dark Current in the CLIC Structure and Muon Cooling Cavity using Track3P

Lixin Ge ACD

Liling Xiao, Zenghai Li

Accelerator Directorate, SLAC

Presented at ICAP09, Sept.03, 2009

Courtesy of Cho Ng, Lixin Ge

Courtesy of Cho Ng, Lixin Ge

Fields enhanced around slot roundin(SLAC

Electron Trajectory & Impact Energy

At 85 MV/m gradient, energy of dark current electrons can reach ~0.4 MeV on impact

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... some other "cavity" type. Hope, you feel better.

Wilhelm Busch: Max und Moritz, sometimes in the 19th century. Widely published http://upload.wikimedia.org/wikipedia/commons/thumb/c/c2/Max_und_Moritz_(Busch)_026.png/800px-Max_und_Moritz_(Busch)_026.png

These are greetings of my co-author Hans-Walter Glock