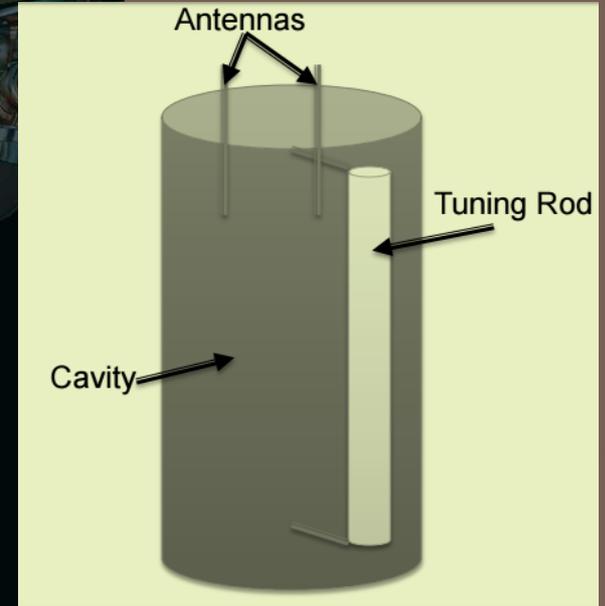
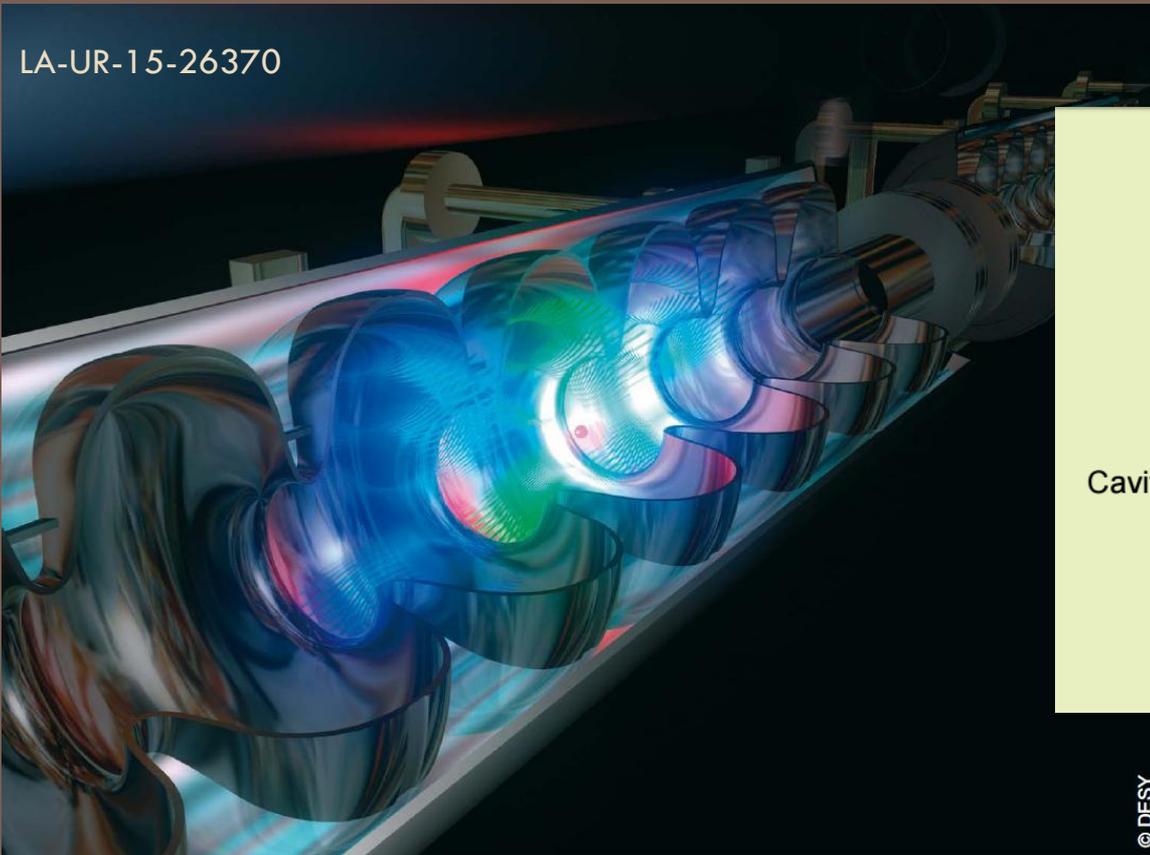


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INTRODUCTION TO RF-STRUCTURES AND THEIR DESIGN – NUMERICAL DESIGN TOOLS – SOME CONSIDERATION OF RF-DETECTOR DESIGNS

Frank L Krawczyk
LANL, AOT-AE, January 2017

Abstract

Introduction to RF-Structures and Their Design
Chapter 4: Numerical Design Tools
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The numerical design chapter of the class addresses two topics: (1) Numerical Methods that include resonator design basics, introduction to Finite Difference, Finite Element and other methods, and (2) Introduction to Simulation Software that covers 2D and 3D software tools and their applicability, concepts for problem descriptions, interaction with particles, couplers, mechanical and thermal design, and finally a list of tips, tricks and challenges.

TOC

□ Design Tools

▣ Numerical Methods

- Resonator design basics
- Basics of Finite Difference and Finite Element Methods
- Other methods

▣ Software

- 2D software
- 3D software
- General concepts of problem descriptions
- Interaction with particles, couplers, mechanical and thermal design
- Tips, tricks and challenges

Numerical Methods

□ Design Basics

- ▣ There is a large number of numerical design tools available addressing a wide range of methods and needs
- ▣ RF-structures with few exceptions cannot be designed analytically
- ▣ The design task: obtain a geometry that can contain or transport electro-magnetic (EM) fields with specific properties
- ▣ Beyond the basic EM properties, designs might consider secondary properties and additional conditions (mechanical, thermal, interaction with charged particles)

Numerical Methods

□ Design Basics

▣ Design of resonating structures

- Pill-box/Elliptical resonators
- Quarter-wave, half-wave or PBG resonators
- RF-gun cavities
- Waveguides (common are rectangular or coaxial guides)

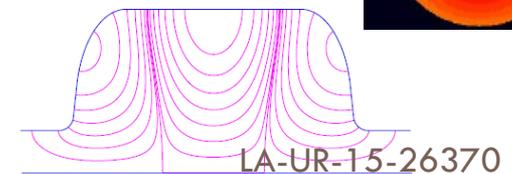
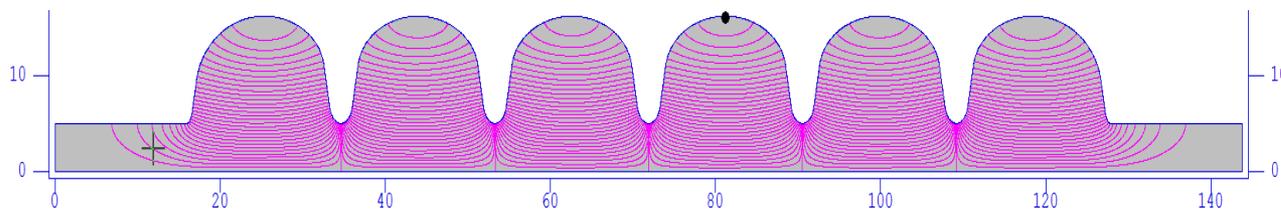
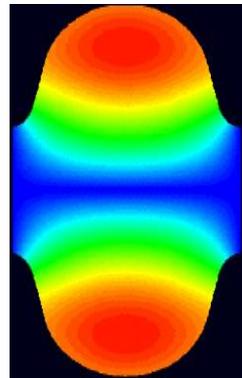
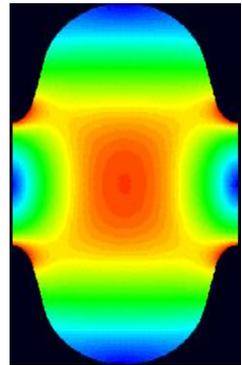
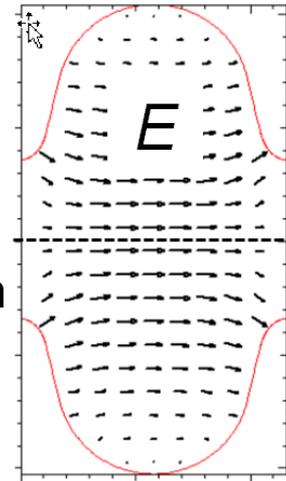
▣ Mathematical problem: Solution of Maxwell's Equations

- for eigenvalues and eigenvectors (Helmholtz)
- for a time-harmonic drive (Helmholtz)
- fully time-dependent (Faraday & Ampere's Law)

Numerical Methods

□ Relevant properties – primary, direct result of the simulation

- Cavity eigenmode frequencies
- Electric & magnetic field patterns of modes
- Application mode (acceleration/interaction)
- Higher/lower order modes (HOM/LOM)
deflecting, specific mode band, “full” spectrum
- Peak surface fields (electric and magnetic)
- Peak surface field locations
- Waveguides: propagation constant, multi-pacting



Numerical Methods

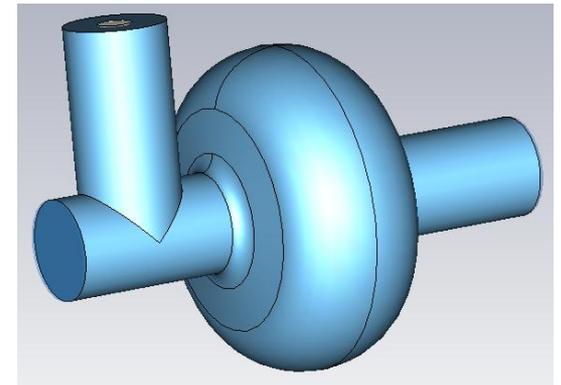
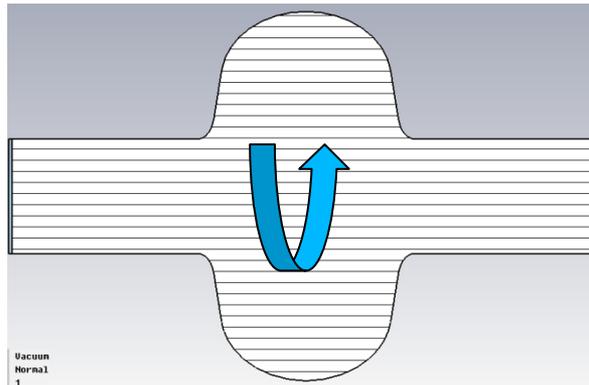
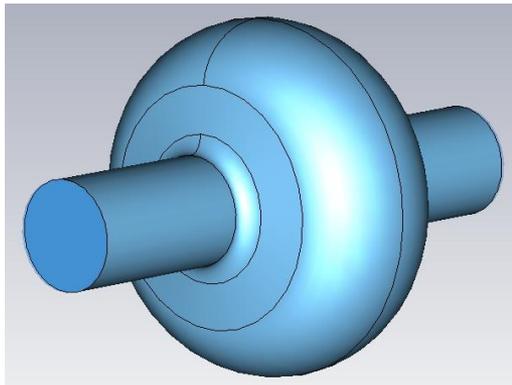
- Relevant properties – secondary, require post-processing steps based on the primary results
 - Resonator losses P_c and loss distribution
 - Quality factor $Q = \omega U / P_c$
 - “Accelerating” voltage $\sim \mathbf{E} \cdot \mathbf{g}, \mathbf{v} \times \mathbf{B} \cdot \mathbf{g}$ (interaction)
 - Transit time factor T (interaction)
 - Shunt Impedance $(V \cdot T)^2 / P_c$
 - Coupling properties (cell-to-cell or to coupler)
 - Tuning sensitivity

Numerical Methods

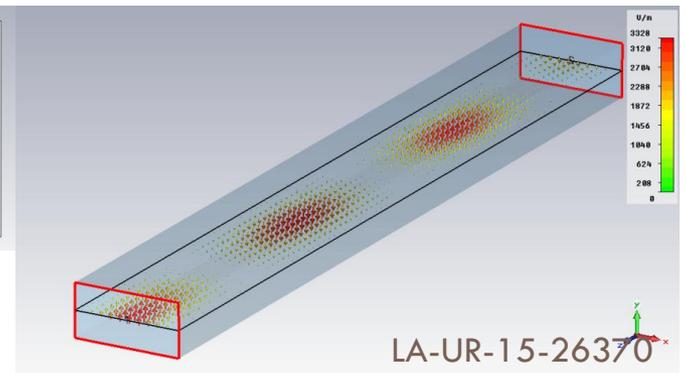
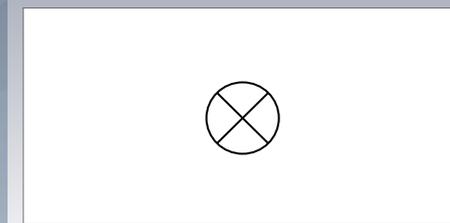
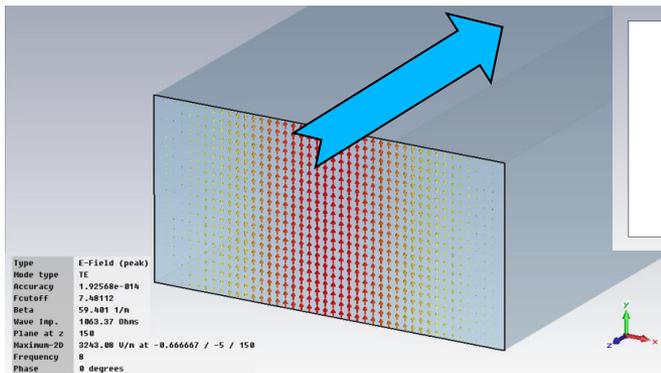
- The selection of design software needs to consider the simulation results you are aiming for
 - ▣ Type of structure
 - ▣ Symmetries
 - ▣ Materials involved
 - ▣ Details of RF-properties needed
 - ▣ Interaction with other structures (e.g. couplers, tuners)
 - ▣ Interaction with other physics characteristics
 - Mechanical, Thermal, Static Fields, Particles

Numerical Methods

- Selection of calculation domain (2D vs. 3D)
 - Azimuthal symmetry (for structure + restrictions for solutions)



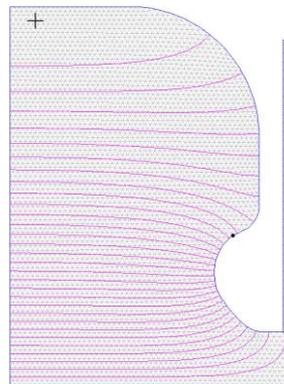
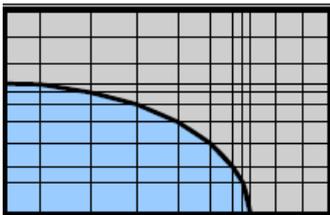
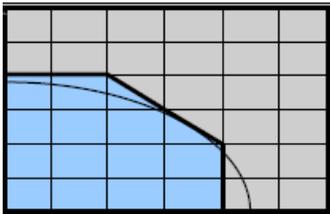
- Translational symmetry (for structure + restrictions for solutions)



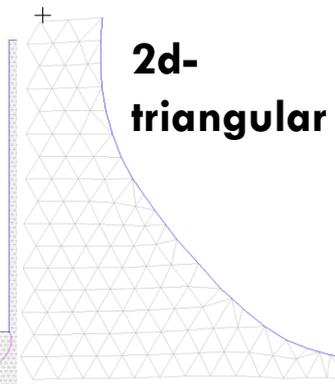
Numerical Methods

- Discretization of the calculation domain: Cartesian, triangular, tetrahedral, regular or unstructured grid, sub-gridding

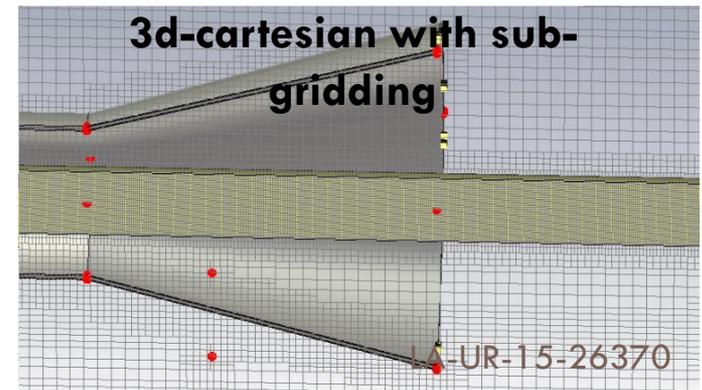
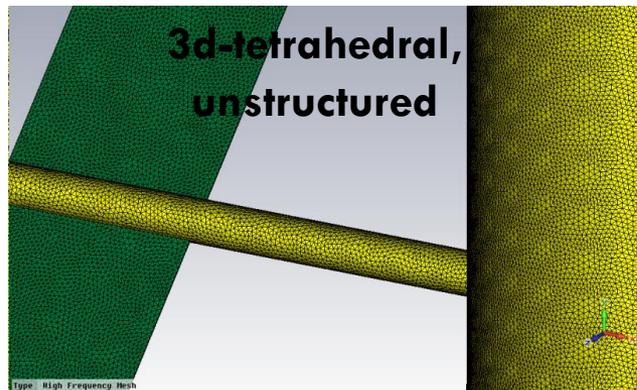
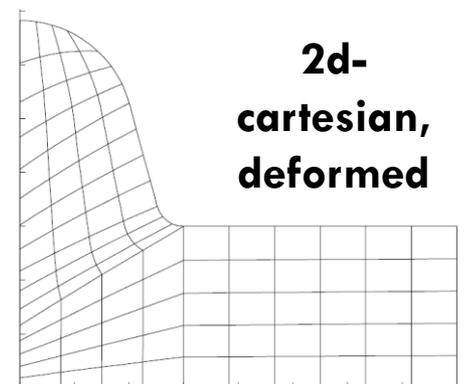
Quality of representation



2d-
triangular



2d-
cartesian,
deformed

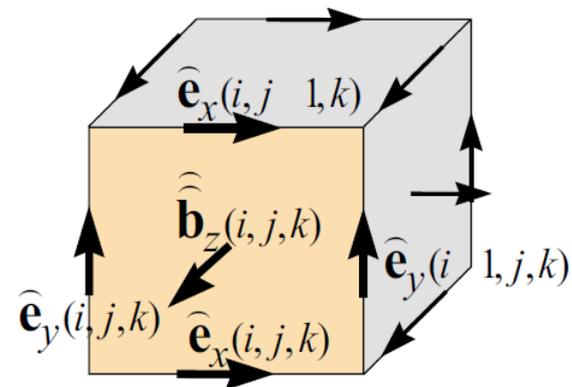
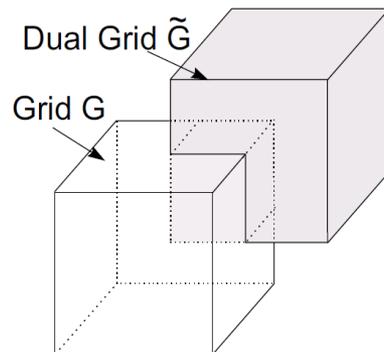


Numerical Methods

- Formulation of Maxwell's equations in discrete space
- Continuous equations will be translated into matrix equations that are solved numerically
- Methods vary in
 - ▣ Discretization of space
 - ▣ Discretization of field functions
 - ▣ Consideration of *surfaces, volumina, solution space, exclusion areas*
 - ▣ Roles of boundaries
 - ▣ Locations of the allocation of solutions: *points, edges, volumina*
 - ▣ Support of modern computer architectures (vector, parallel, multi-core, ...)

Numerical Methods

- Finite Difference (FD) or Finite Integration (FIT):
 - Differential or integral operators are replaced by difference operators
 - Equations couple values in neighboring grid elements
 - → often regular elements, sparse banded matrices
 - quality of surface approximations depends on software implementation
 - Allocation of the fields in the discrete space (YEE algorithm)



Numerical Methods

□ Differential operators

1st derivative

$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i+1} - u_i}{\Delta x} \quad \text{forward difference}$$

$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_i - u_{i-1}}{\Delta x} \quad \text{backward difference}$$

$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x} \quad \text{central difference}$$

2nd derivative

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} + \mathcal{O}(\Delta x)^2$$

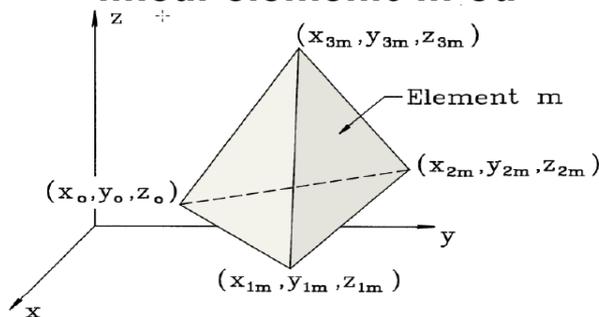
- Coupling between elements provided by common points
- Coefficients include material properties along edges/surfaces
- Solutions minimize local energy integral in each cell
- Special FIT properties: difference operators fulfill discrete vector-analytic operators (e.g. $\text{curl grad} \equiv 0, \dots$)

Numerical Methods

□ Finite Elements (FE):

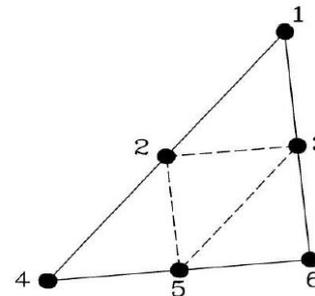
- Differential or integral operators act on discrete approximations of the field functions (base polynomials of low order)
- → regular or irregular elements, banded matrices, sparseness depends on element type
- mostly superior surface representation

Representation of field with linear elements in 3d



$$\mathbf{E}_m = \alpha_{1m}\mathbf{X} + \alpha_{2m}\mathbf{Y} + \alpha_{3m}\mathbf{Z}.$$

Representation of field with second order elements in 2d



$$\phi(x, y) = a_0 + a_1x + a_2y + a_3x^2 + a_4xy + a_5y^2.$$

Numerical Methods

- Coupling between elements provided by common points
- Coefficients include material properties along edges/surfaces
- Solutions minimize global energy integral in calculation volume
- Increased order reduces number of required elements for a given accuracy, but might reduce sparseness of matrices

- Suggested Reading:
 - FD: Allan Taflove, Susan Hagness, Computational Electrodynamics: The Finite Difference Time Domain Method, 3rd Edition (2005)
 - FIT: Thomas Weiland, Marcus Clemens:
<http://www.jpier.org/PIER/pier32/03.00080103.clemens.pdf>
 - FEM: Stan Humphries:
<http://www.fieldp.com/femethods.html>

Numerical Methods

- Other Methods
 - **Boundary Integral Methods** or **Method of Moments**: Continuous volume solutions from sources on discretized metal surfaces
 - **Transmission Line Matrix**: Solving resonator problems as lumped circuit models
 - **Scattering Matrix Approaches**: Quasi optical approach based on diffraction from small features
 - Specialized solvers for *fields inside conductors* (metals/plasmas)
 - Specialized solvers *merging optical systems with regular RF-structures* (e.g. Smith-Purcell gratings)

Software Tools - 2D

- The Superfish family of codes
(<http://laacg.lanl.gov/laacg/services/>)
 - ▣ *2d (rz, xy), FD, triangular, TM (TE), losses, post-processing, part of general purpose suite*
- The Superlans codes (D.G.Myakishev, V.P.Yakovlev, Budker INP, 630090 Novosibirsk, Russia)
 - ▣ *2d (rz, xy), FE, quadrilateral, TM, losses, post-processing*
- The codes from Field Precision
(<http://www.fieldp.com/>)
 - ▣ *2d (rz, xy), FE, triangular, TM/TE, losses, some post-processing, part of general purpose suite*

Software Tools - 2D

- 2D modules of MAFIA (or even older versions like URMEL, TBCI, ...)
 - ▣ *2d (rz, xy), FIT, Cartesian, TM/TE, losses, post-processing, general purposes suite, PIC and wakes*
 - ▣ these are not distributed anymore, but still used at accelerator laboratories

While 2D codes were the standard up to 10 years ago, their use is decreasing. Their strength is speed and accuracy. One strong reason for those codes is the design of SRF elliptical resonators, where peak surface fields are of importance.

Software Tools - 3D

- MAFIA (<http://www.cst.com/>)
 - ▣ 2d/3d (xy, rf, xyz, rfz), FIT, Cartesian, losses, post-processing, general purpose suite, PIC & wakes
 - ▣ Historically, MAFIA was the first 3d general purpose package for design of accelerator structures
- GdfidL (<http://www.gdfidl.de/>)
 - ▣ 3d (xyz), FIT, Cartesian, losses, post-processing, general purpose suite, wakes, HPC support
- CST Microwave Studio (<http://www.cst.com/>)
 - ▣ 3d (xyz), FIT/FE, Cartesian/tetrahedral, losses, post-processing, general purpose suite, PIC & wakes, thermal, HPC support
- HFSS (<http://www.ansoft.com/products/hf/hfss/>)
 - ▣ 3d (xyz), FE, tetrahedral, losses, post-processing, general purpose suite, interface to mechanical/thermal, HPC support

Software Tools - 3D

- Analyst (<http://web.awrcorp.com/Usa/Products/Analyst-3D-FEM-EM-Technology/>)
 - ▣ 3d (xyz), FE, tetrahedral, losses, post-processing, HPC support, wakes
- Comsol (<http://www.comsol.com/>)
 - ▣ 3d (xyz), FE, tetrahedral, losses, post-processing, part of a multi-physics suite including mechanical/thermal and beyond
- Vorpal (<http://www.txcorp.com/products/VORPAL/>)
 - ▣ 3d (xyz), FE, tetrahedral, losses, post-processing, particles & wakes, HPC support
- Remcom Codes (<http://www.remcom.com/>)
 - ▣ 3d (xyz), FD, Cartesian, losses, post-processing, HPC support

Software Tools - 3D

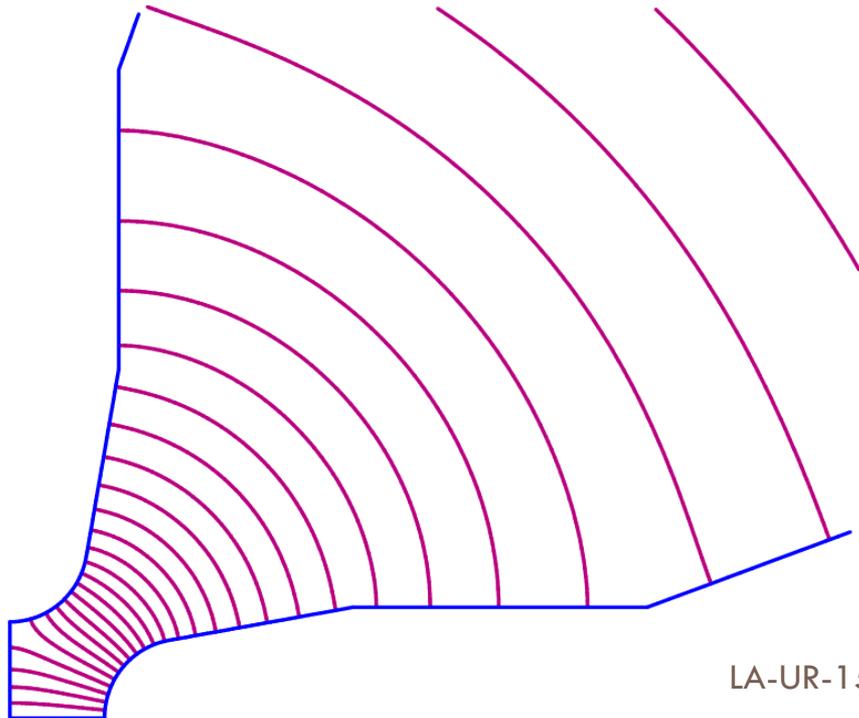
- SLAC ACE3P
(<http://www.slac.stanford.edu/grp/acd/ace3p.html>)
 - 3d (xyz), FE, tetrahedral, losses, post-processing, PIC & wakes, HPC support
- The strengths of 3D codes
 - Treatment of complex geometries
 - Support of general CAD formats
 - Flexible post-processing
 - Professional interfaces and design controls but they are slower and need much more expensive resources
- Links to more software
 - <http://emclab.mst.edu/csoft.html>
 - <http://www.cvel.clemson.edu/modeling/EMAG/csoft.html>

Software Tools – Problem Definition

□ Resonator geometry

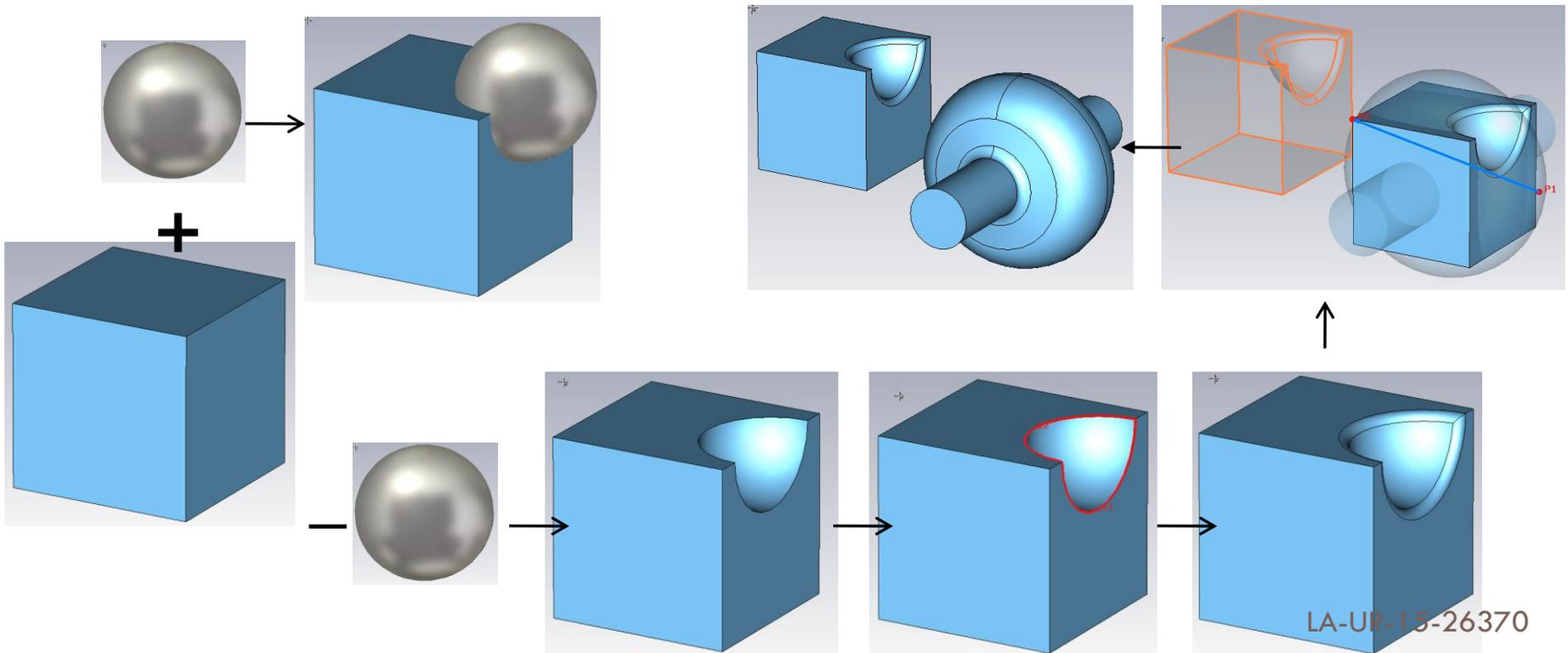
- 2d: polygons describe contours, straight-forward for linear segments, cumbersome for curved polygons, most codes do not allow use of parameters

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&po nt=2,x0=0.54071,y0=0.,x=-.24371,y=0. &  
&po x=0.,y=0. &
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Software Tools – Problem Definition

- 3d: assembly of primitives with Boolean superposition, CAD style tools that allow definition of separate sub assemblies, import/export of CAD models, blends, extrusions,



Software Tools – Problem Definition

□ Material properties

- For RF-properties only the interior of resonators needs to be modeled
- In general the outside space will be assigned the properties of the metallic enclosure
- Enclosing metals only required for thermal/mechanical considerations, for a mix of metals, or for internal features
- Dielectric or permeable inclusions, like rf-windows, ferrites, ... will need to be added
- Perfect conductors and non-lossy dielectrics are standard
- Newer codes also allow permeable and lossy properties
- Few rf-codes handle non-linear materials (except for magnetostatics codes)

Software Tools – Problem Definition

- Material properties
 - ▣ Losses in dielectrics and ferrites need to be considered during the resonator evaluation. They require appropriate complex solvers
 - ▣ Treatment of losses in metals is a special case
 - For rf-resonators loss-considerations do not need modeling of the skin-depth layer of the metal
 - Explicit consideration of losses is handled by the modeling software
 - For most codes it is suggested to assume perfect conducting metals for the field solutions (does not require complex solvers). The rf-losses are calculated in a post-processing step from the bulk resistivity and the surface magnetic fields

Software Tools – Problem Definition

- Boundary conditions
 - ▣ PDE solutions require specifications of solutions at the volume boundaries. For the solution of Maxwell's Equations the conditions are given by the physical problem. Common conditions are
 - Dirichlet: Constant potential or vanishing tangential field
 - Neumann: Constant potential derivative or vanishing normal field
 - Mixed: combined Dirichlet and Neumann conditions (uncommon)
 - ▣ In (often) rectangular calculation volumes, boundary conditions on each surface can be chosen to be different
 - ▣ For the definition one needs to be aware, if the specification is for the electric or magnetic field properties on the boundary

Software Tools – Problem Definition

□ Boundary conditions

- Waveguide ports: Waveguides connected to resonators can be modeled by short longitudinally invariant sections. Their terminations are modeled as an impedance-matched layer. This boundary condition is important for evaluation of resonator -coupler interaction
- Open boundaries: Simulation of solutions radiating into open space. The methods depend on the physics problem. Methods used are *solutions expansions*, *absorbing boundary conditions*, or *Perfectly Matched Layers (PML)*, an improved type of absorbing condition less prone to frequency or angle of incidence

Software Tools – Problem Definition

- Besides the descriptions relevant to the rf-structure, there is a number parameters that need to be set before a simulation can be performed. These include
 - ▣ Problem-type
 - ▣ Meshing controls
 - ▣ Frequency estimate (for meshing or for time-harmonic solvers)
 - ▣ Some beam properties (for transit-time factors and other secondary properties, for parametric generators of special geometries like elliptical resonators)
 - ▣ Solver type and configurations, ...

Software Tools – More Features

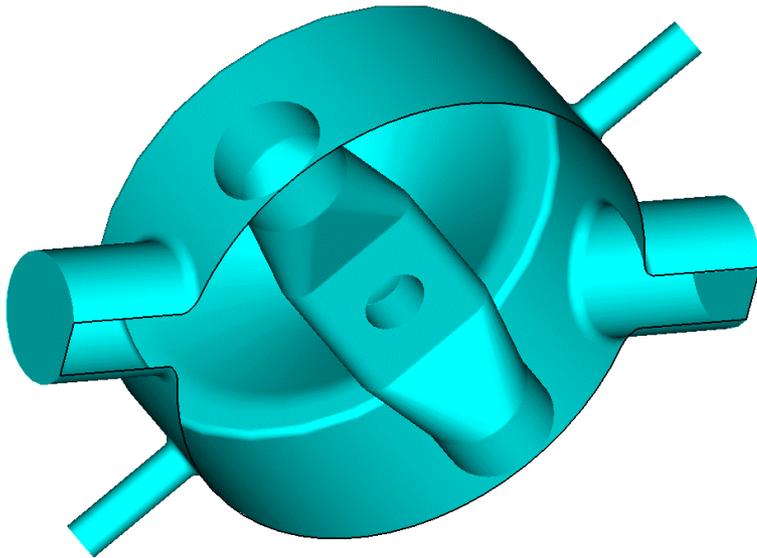
- Parameterization: flexible description of geometries allows for better design strategies and optimization (most 3D codes)
- Optimization: User defined goals and strategies can be defined in many 3d suites, some support in 2d
- Post-processing: All codes listed support basic post-processing in the form of solution display and calculation of secondary quantities relevant to accelerator applications. Some 3d-suites allow additional user-defined post-processing
- Parallel software: The need for larger resources led to the addition of solvers that support massively parallel computations (multi-core, MPI, GPUs)

Interaction with Mechanical/Thermal Design

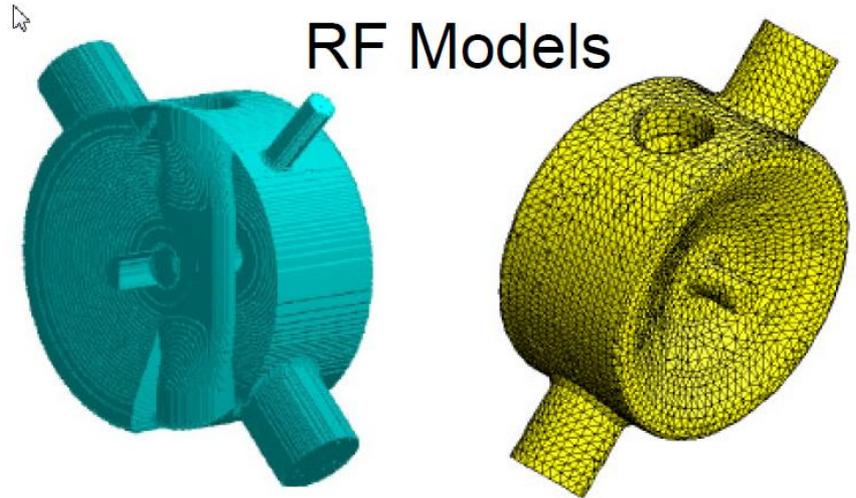
- RF-designs are not stand-alone, feasibility of fabrication, mechanical stability and thermal loads needs to be considered also
- General purpose and multi-physics tools permit evaluation of several aspects without a complete re-build for each domain of evaluation
- ***Note however: EM fields require meshing of enclosed volume, thermal/mechanical properties require meshing of enclosure, this needs to be considered during the structure generation***
- Effects due to mechanical deformations are small, one needs to pay attention that effects are real and not driven by discretization errors

Interaction with Mechanical/Thermal Design

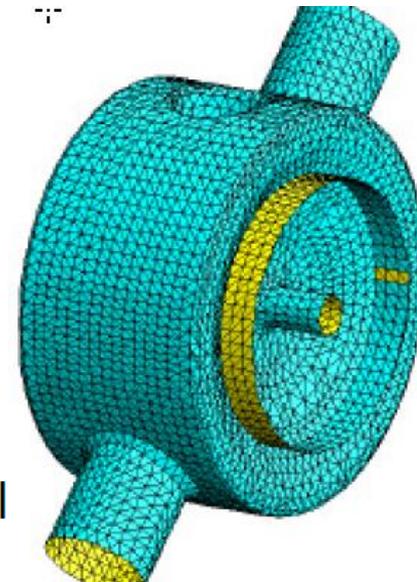
Common CAD Model



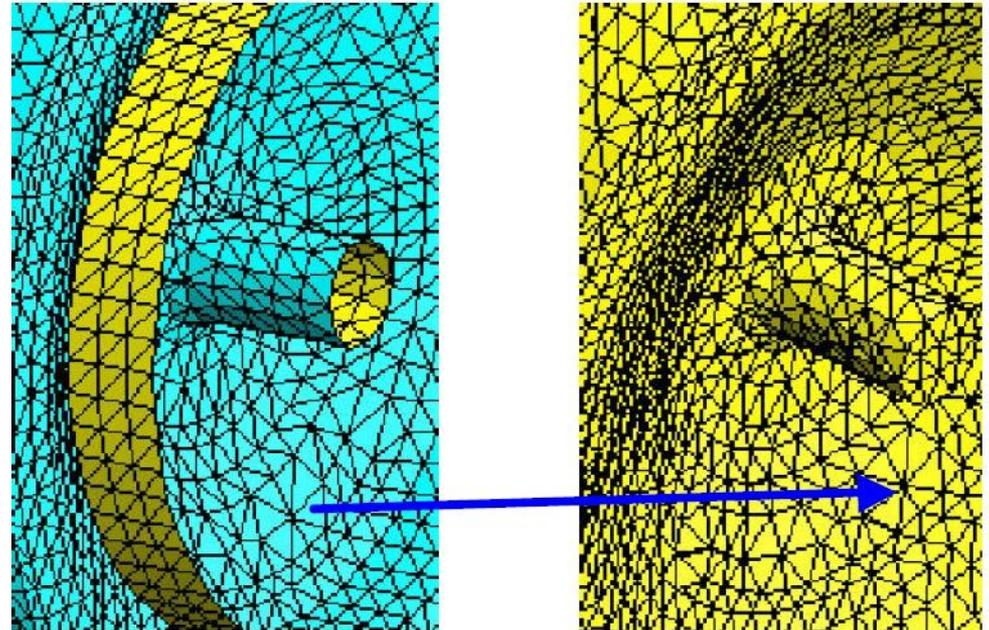
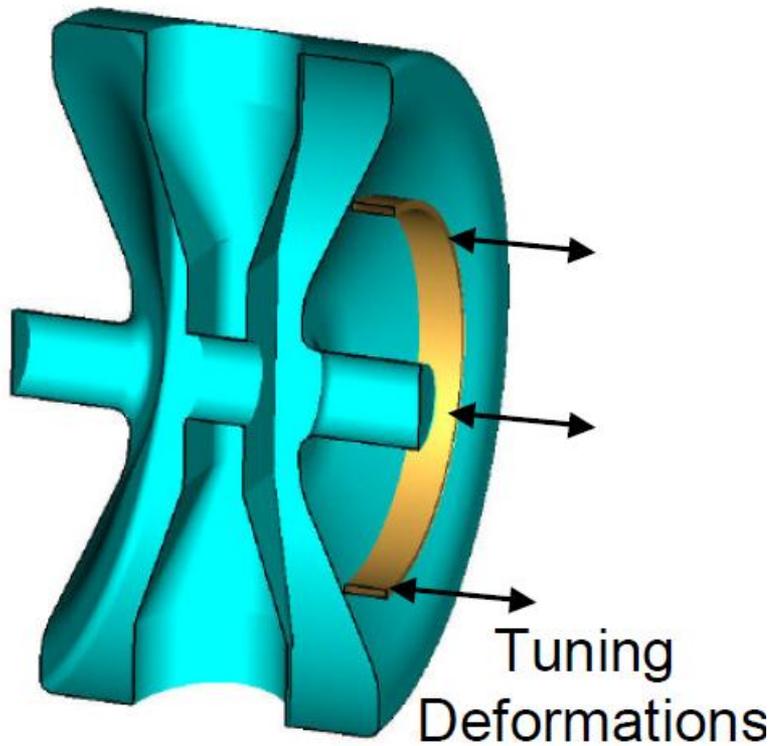
RF Models



Structural Shell Model



Interaction with Mechanical/Thermal Design



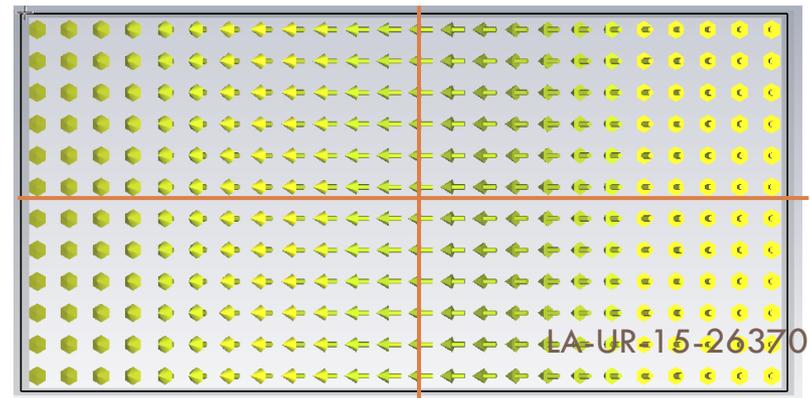
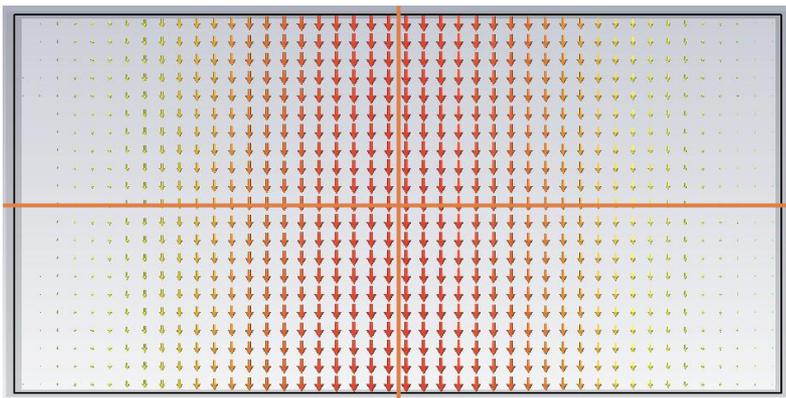
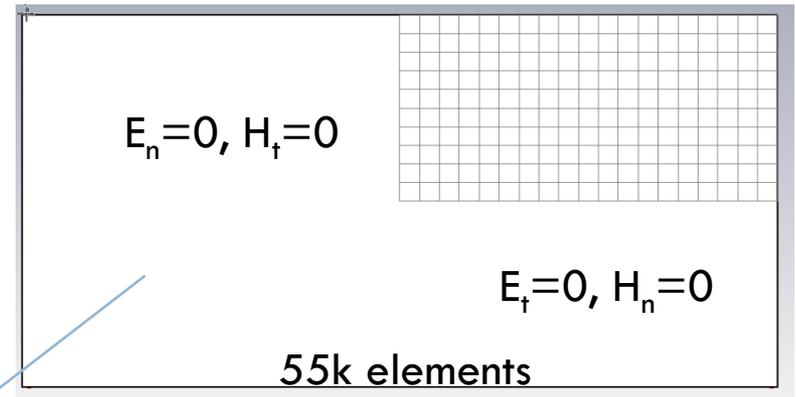
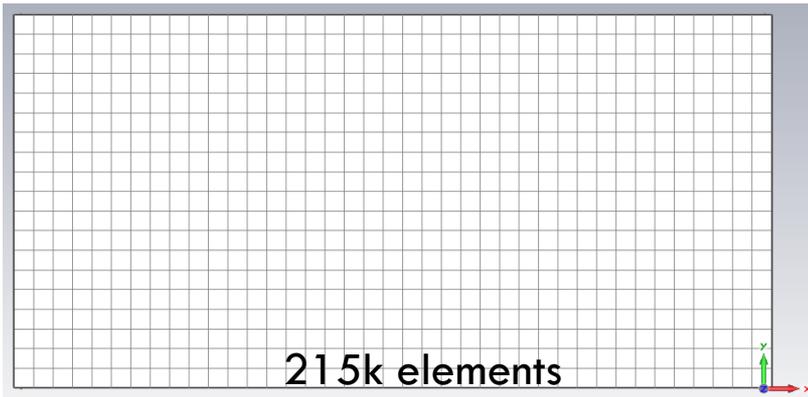
Shell Mesh ↔ Volume Mesh
Common nodes allow recalculation
of RF-case without re-meshing
(reduces discretization error)

Numerical Challenges

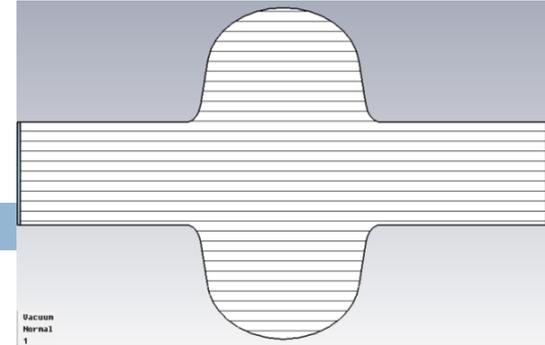
- Feature rich software is mostly full 3D, which makes structure development slow. Where 2D would not suffice – consider parallel versions
 - ▣ Several of the 3D codes support solver versions on high performance computing platforms.
 - ▣ The minimum support is for multiple cores in standard cpus.
 - ▣ There are also versions for clusters (using mpi) or for using GPUs.
 - ▣ Analyst, ACE3P, Vorpak are predominantly written for HPC platforms

Tips and Tricks

Use of symmetries: Boundary conditions cannot only be used to define the properties at the outside of a problem. They can also be used to reduce problem size or enforce finding specific modes



Tips and Tricks



- Beam pipe modeling: Basic rf-design for SRF-structures often requires modeling of resonators with open beam-pipes. Standard boundary conditions are only approximately correct. Open boundaries are often not supported for eigenvalue solvers. To estimate, if a beam-pipe is long enough to not affect the solution, the following approach is suggested:
 - ▣ Calculate twice, once with Dirichlet and once with Neumann conditions. The change in frequency should be very small
 - ▣ Add a metal (flange) on the pipe-end. Calculate Q with and without the losses in the termination. If the Q-change in $< 1\%$ this is also a good position for testing a cavity

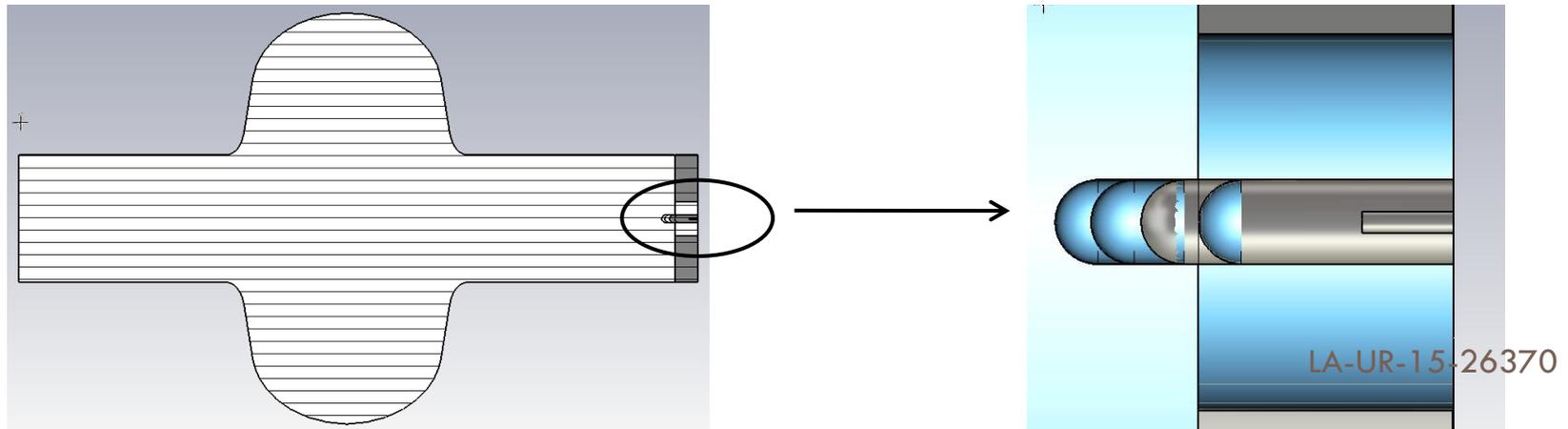
Tips and Tricks

- Tuning sensitivities: Frequency changes from small changes in geometry need to be determined. Those might not be very accurate, as the discretization errors can dominate the solutions. Some solutions:
 - Model a few larger changes, check if the sensitivity behaves linear
 - Use expert system meshers, those for small changes in geometry only move element nodes to new positions without remeshing
 - Use Slater's Perturbation Theorem (also useful for LFD and surface removal)

$$\frac{\Delta\omega}{\omega} = \frac{\int_{\Delta V} (\mu_0 H^2 - \epsilon_0 E^2) dV}{\int_{\Delta V} (\mu_0 H^2 + \epsilon_0 E^2) dV} = \frac{\Delta U_m - \Delta U_e}{U}$$

Tips and Tricks

- Dealing with small changes in geometry:
 - ▣ Determination of the external Q (coupling) for a coupler attached to a resonator.
 - ▣ Determination of changes by moving tuning devices.
 - ▣ To avoid errors due to the change in discretization the following strategy works well:
 - ▣ Model different positions of a substructure simultaneously, only changing material properties, this preserves meshing



Tips and Tricks

- Meshing: Many codes use auto mesh generators that fulfill certain criteria. For those who do not provide auto-meshing or for control of special circumstances some rules should be kept in mind:
 - Consider the highest frequency relevant for a simulation and make sure that your mesh uses at least 10 steps per wavelength at this frequency.
 - For the typically low operation frequency problem can be made small, keep in mind that calculation of HOMs increases the required density
 - For interaction with particles, especially for wake fields of ultra-short bunches, meshing needs to extremely fine (e.g. for a bunch-length of 1 mm (rms) the highest bunch frequency is 177 GHz)
 - PIC codes often require equidistant meshes

The End

Thanks to the community from which I borrowed examples and illustrations

As I do not credit any providers, please refrain from using these materials outside this meeting

I can provide references for specific topics if needed