Simulation packages and Review of Codes

Alexej Grudiev
CERN, BE-RF
Packages for computer simulations of electromagnetic EM fields and more

- CST
- GdfidL
- HFSS
- ACE3P
- COMSOL
CST Studio Suite

CST STUDIO SUITE:
- **CST MWS**
- CST DS
- CST EMS
- **CST PS**
- CST MPS
- CST PCBS
- CST CS
- CST MICROSTRIPES
- Antenna Magus
CST: All(?) you need in one package

• Powerful and user-friendly Input:
  • Probably the best time domain (TD) solver for wakefields or beam coupling impedance calculations (MAFIA)
    • Beta < 1
    • Finite Conductivity walls
  • Once geometry input is done it can be used both for TD and FD simulations
  • Moreover using Design Studio (DS) it can be combined with the other studios for multiphysics and integrated electronics simulation, but this is relatively fresh fields of expertise for CST
  • Accelerator physics oriented post processor, especially in MWS and PS
  • Enormous progress over the last few years compared to the competitors.

An example of what can be solved easily on a standard PC

Courtesy of Igor Syratchev
CST (examples)

Two examples of what can be solved on bigger PC:
128 GB of RAM and 24 CPUs

CLIC accelerating structure from Cu with
HOM damping loads from SiC
(frequency dependent properties)
CST (examples)

Transverse wake at offset of 0.5 mm

Transverse beam coupling impedance at offset of 0.5 mm
CST (examples)

LHC TDI 5m long with ferrite

Benoit Salvant
CST MWS: Comparison with HFSS

(Praveen Ambattu, Vasim F. Khan)

<table>
<thead>
<tr>
<th>Property</th>
<th>MWS (PEC)</th>
<th>HFSS (Cu)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freq, GHz</td>
<td>11.9941</td>
<td>11.9959</td>
</tr>
<tr>
<td>$Q_{Cu}$</td>
<td>6395</td>
<td>6106</td>
</tr>
<tr>
<td>$R_t/Q$, Ohm</td>
<td>54.65</td>
<td>53.78</td>
</tr>
<tr>
<td>$E_{surf}/E_t$</td>
<td>3.43</td>
<td>3.28</td>
</tr>
<tr>
<td>$H_{surf}/E_t$</td>
<td>0.0114</td>
<td>0.0106</td>
</tr>
</tbody>
</table>

- MWS used Perfect Boundary Approximation, 134,912 hexahedra per quarter (lines/lambda=40, lower mesh limit=40, mesh line ratio limit=40)
- HFSS used 8,223 tetrahedra per quarter (surface approximation= 5µm, aspect ratio=5)
CST MWS: Example. S-parameters in CLIC Crab cavity

Mesh view

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material</td>
<td>Copper (annealed)</td>
</tr>
<tr>
<td>Type</td>
<td>Lossy metal</td>
</tr>
<tr>
<td>E1. cond.</td>
<td>$5.8 \times 10^7$ [S/m]</td>
</tr>
<tr>
<td>Rho</td>
<td>8930 [kg/m$^3$]</td>
</tr>
<tr>
<td>Therm.cond.</td>
<td>401 [W/K/m]</td>
</tr>
<tr>
<td>Young's Mod.</td>
<td>120 [kN/mm$^2$]</td>
</tr>
<tr>
<td>Polss.Ratio</td>
<td>0.33</td>
</tr>
<tr>
<td>Thermal Exp.</td>
<td>17 [1e-6/K]</td>
</tr>
</tbody>
</table>

- Type: Powerflow (peak)
- Monitor: power (f=11.9942)
- Component: Abs
- Plane at x: Θ
- Maximum-2D: 35709.6 VA/m$^2$ at Θ / 5.4859 / 92.5097
- Frequency: 11.9942

(Praveen Ambattu)
CST: Shortcomings

1. **Cartesian mesh**: Especially in FD can results to less accurate calculations of **frequency, Q-factor, surface fields** compared to tetrahedral mesh (HFSS, COMSOL, ACE3P). Tetrahedral mesh became available only recently but it is improving very rapidly.

2. Boundary conditions can be set only in Cartesian planes

3. No Field Calculator (HFSS)

4. From three eigenmode solvers only one takes into account losses but it is iterative and very slow

5. ...

With a great help of Andrei Lunin
HFSS: Still an excellent tool for FD

High-Performance Electronic Design
- Ansoft Designer
- ANSYS HFSS
- ANSYS Q3D Extractor
- ANSYS SItwave
- ANSYS TPA

Electromechanical Design
- ANSYS Multiphysics
- ANSYS Maxwell
- ANSYS Simplotter
- ANSYS PExptr
- ANSYS RMxpert

Product options
- AnsoftLinks for ECAD
- AnsoftLinks for MCAD
- ANSYS Distributed Solve
- ANSYS Full-Wave SPICE
- ANSYS Optimetrics
- ANSYS ParICs

• HFSS was and I think still is superior tool for FD simulations both S-pars and eigenmode, though CST shows significant progress in the recent years
• Automatic generation and refinement of tetrahedral mesh
• Most complete list of boundary conditions which can be applied on any surface
• Ansoft Designer allows to co-simulate the pick-up (antenna), cables plus electronics and together with versatile Optimetrics optimise the design of the whole device
• Last year HFSS become a integral part of ANSYS – reference tool for thermo-mechanical simulations -> multiphysics
• Last year time-dependent solver has been released
LHC TDI 5m long beam dump:
One of the most dangerous eigenmodes at 1.227 GHz, $Q = 873$,
Tetrahedral mesh with mixed order ($0^{th}$, $1^{st}$, $2^{nd}$) elements: $N_{tet} = 1404891$
Solution obtained on a workstation with 128 GB of RAM,
HFSS (example, S-parameters)

Port excitation

Incident plane wave excitation

Inverse FFT

O. Kononenko

Frequency Response [kV W⁻¹/²]

Beam Impedance [V / mA]

Time Response [V W⁻¹/²/s]

Wake Potential [V / pC]

Frequency [GHz]
Example
Antenna with matching circuitry

Nominal Requirements
Create matching circuitry between RF PA and antenna

Procedure
1. Analyze Antenna in HFSS
2. HFSS model can be parameterized needed
3. Dynamically link HFSS sub-model results into Designer
4. Create general matching and driving circuitry in Designer
5. Tune/optimize matching circuitry.

Benefit
1. Matching network can be designed schematic with realistic frequency varying load attached (active model)
2. Model is tunable.
3. Engineer has visual indication of performance while tuning/optimizing it.
4. Design is ready for harmonic balance analysis in Nexxim.

HFSS example
HFSS: shortcomings

1. No possibility to simulate particles
2. Automatic mesh is not always perfect, but it has improved after adoption by ANSYS
3. TD and multiphysics are only recently implemented, but thermo-mechanics from ANSYS is a reference by itself
4. ...
The GdfidL Electromagnetic Field simulator
GdfidL computes electromagnetic fields in 3D-structures using parallel or scalar computers.

GdfidL computes
- Time dependent fields in lossfree or lossy structures. The fields may be excited by
  - port modes,
  - relativistic line charges.
- Resonant fields in lossfree or lossy structures.
- The postprocessor computes from these results eg. Scattering parameters, wake potentials, Q-values and shunt impedances.

Features
- GdfidL computes only in the field carrying parts of the computational volume. For eg. waveguide systems, this makes GdfidL about three to ten times faster than other Finite Difference based programs.
- GdfidL uses generalised diagonal fillings to approximate the material distribution. This reduces eg. the frequency error by about a factor of ten.
- For eigenvalue computations, GdfidL allows periodic boundary conditions in all three cartesian directions simultaneously.
- GdfidL runs on parallel and serial computers. GdfidL also runs on clusters of workstations.

Availability
- GdfidL only runs on UNIX-like operating systems.

Price
The price for a one year license for the serial version of GdfidL (including support) starts at 10.000 Euro. The price for a one year license for the parallel versions starts at 20.000 Euro. Access to a powerful cluster where GdfidL is installed on costs 9.000 Euro per year.

Powerful Syntax  Material Approximation  Absorbing Boundary Conditions  Periodic Boundary Conditions
CLIC accelerating structure from Cu with HOM damping loads from SiC (frequency dependent properties)
GdfidL: shortcomings

1. Available only under UNIX-like systems
2. Geometry input is limited
3. It is ‘one man show’
4. ...

<table>
<thead>
<tr>
<th>COMSOL Multiphysics®</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>AC/DC Module</strong></td>
<td><strong>Heat Transfer Module</strong></td>
<td><strong>CFD Module</strong></td>
<td><strong>Chemical Reaction Engineering Module</strong></td>
<td><strong>Optimization Module®</strong></td>
<td><strong>LiveLink™ for MATLAB®</strong></td>
</tr>
<tr>
<td><strong>RF Module</strong></td>
<td><strong>Structural Mechanics Module</strong></td>
<td><strong>Microfluidics Module</strong></td>
<td><strong>Batteries &amp; Fuel Cells Module</strong></td>
<td><strong>Material Library</strong></td>
<td><strong>LiveLink™ for SolidWorks®</strong></td>
</tr>
<tr>
<td><strong>MEMS Module</strong></td>
<td><strong>Geomechanics Module</strong></td>
<td><strong>Subsurface Flow Module</strong></td>
<td><strong>Electrodeposition Module</strong></td>
<td><strong>Particle Tracing Module</strong></td>
<td><strong>LiveLink™ for Pro/ENGINEER®</strong></td>
</tr>
<tr>
<td><strong>Plasma Module</strong></td>
<td><strong>Acoustics Module</strong></td>
<td></td>
<td></td>
<td></td>
<td><strong>LiveLink™ for Inventor®</strong></td>
</tr>
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<td></td>
<td><strong>LiveLink™ for AutoCAD®</strong></td>
</tr>
</tbody>
</table>
COMSOL: example \( \frac{df}{dp} \) Calculation

**Electromagnetic Waves**
- Solving only for the RF domain
- Applying the prober boundary conditions

**Solid Mechanics**
- Solving only for the Cavity Vessel
- Applying the proper fixed constraints, symmetries, displacements, and boundary load

**Moving Mesh**
- Solving for all domains
- Applying the proper prescribed and free mesh deformation/displacement

**Three Multiphysic Modules**

**Two Simulation Studies**

<table>
<thead>
<tr>
<th>Study 1</th>
<th>Study 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eigen-frequency (to find ( f_0 ))</td>
<td>Stationary (solving only for solid mechanics and moving mesh)</td>
</tr>
<tr>
<td></td>
<td>Eigen-frequency (to find ( f_p ))</td>
</tr>
</tbody>
</table>

**Equation**

\[
\frac{df}{dp} \frac{f_p-f_0}{P_L}
\]

Mohamed Hassan
Example

**Electromagnetic Waves**
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Stainless Steel Vessel
Niobium Shell
RF Domain
Symmetry Boundaries
Prescribed Displacement $u,v,w$
$dx=0$
$dy=0$
$dz=0$

PEC
PMC
Fixed Constraint
Pressure Boundary Load
Free Deformation
Mohamed Hassan
Meshes used for RF kick simulations: a) HFSS, b) CST MWS, c) COMSOL

- ‘Highly regularized tetrahedral mesh can be built by versatile COMSOL mesh generator’
- ‘Well parallelized, direct method for eigenmode calculations with losses and smooth surface fields’

Andrei Lunin
COMSOL: shortcomings

• Geometry input is limited
• Port excitation mode description is not convenient
• S-parameter solver is not convenient
• Postprocessing is not well developed at least for what concerns accelerator physicists and engineers

Andrei Lunin
# Accelerator Modeling with EM Code Suite \textbf{ACE3P}

**Meshing** - \textit{CUBIT} for building CAD models and generating finite-element meshes


**Modeling and Simulation** – SLAC’s suite of conformal, higher-order, C++/MPI based parallel finite-element electromagnetic codes


## \textbf{ACE3P (Advanced Computational Electromagnetics 3P)}

<table>
<thead>
<tr>
<th>Domain</th>
<th>Code</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency Domain:</td>
<td>Omega3P</td>
<td>Eigensolver (damping)</td>
</tr>
<tr>
<td></td>
<td>S3P</td>
<td>S-Parameter</td>
</tr>
<tr>
<td>Time Domain:</td>
<td>T3P</td>
<td>Wakefields and Transients</td>
</tr>
<tr>
<td>Particle Tracking:</td>
<td>Track3P</td>
<td>Multipacting and Dark Current</td>
</tr>
<tr>
<td>EM Particle-in-cell:</td>
<td>Pic3P</td>
<td>RF guns &amp; klystrons</td>
</tr>
<tr>
<td>Multi-physics:</td>
<td>TEM3P</td>
<td>EM, Thermal &amp; Structural effects</td>
</tr>
</tbody>
</table>

**Postprocessing** - \textit{ParaView} to visualize unstructured meshes & particle/field data

Accelerator Design and Analysis with ACE3P

Constraint
\[ f = f_0 \]
Maximize \((R/Q, Q)\)
Minimize (surface fields etc.)

Minimize Wakefields

Model CAD → Meshing Cubit → Partitioning ParMetis → Solvers → Visualization ParaView

ACE3P EM Field Computations
Determine Cavity Dimensions

Fabrication
Cell QC
Wakefield Measurement

SLAC
SciDAC
waveguide

CLIC two-beam module rf circuit

PETS

AS

ACE3P: example

Arno Candel et al.,
SLAC-PUB-14439

$ t=02.50 \text{ ns} $

$ t=08.00 \text{ ns} $
ACE3P: shortcomings

• Very complex package to use. It is not user-friendly at all and requires a lots of time to invest before it can be used efficiently

• It is not a commercial product -> no manual reference, limited tech support. No it is an open source.

• ...

Summary

1. CST
   - Larger objects in TD
   - Better FD calculations, 3D EM + circuit co-simulation, RF + thermal + structural
   - More multiphysics

2. GdfidL
   - Accurate solution for very larger objects in TD and FD

3. ANSYS HFSS

4. COMSOL

5. ACE3P