Latest Developments in 3D Charged Particle Simulations

Felix Wolfheimer, CST AG
CST STUDIO SUITE - Overview

CST MICROWAVE STUDIO®
Our Flagship Product for RF Simulations

CST CABLE STUDIO™
CST PCB STUDIO™
CST MICROSTRIPES™

Common Easy-To-Use Pre- and Post-processing Engine

CST DESIGN STUDIO™
Circuit Simulator
Coupling of 3D Models
System Assembly and Modeling

CST PARTICLE STUDIO®
Interaction of EM Fields with Free Moving Charges

CST MPHYSICS STUDIO™
Thermal and Mechanical Effects of EM Fields

CST EM STUDIO®
Simulations of Static or Low-Frequency Fields

RF Simulations for Special Applications
| **Tracking** | Solver for particles in static fields including space charge or in harmonic fields excluding space charge. |
| **Particle In Cell** | Self-consistent transient field and particle solver including full space charge effects at all frequencies. |
| **Wakefield** | Transient solver with special beam excitation (predefined fixed straight beam path) |
Tracking Algorithm

Workflow

1. Calculate electro- and magnetostatic fields.
2. Move particles according to the previously calculated force. Trajectories
3. Adjust trajectories/fields according to space-charge (gun iteration).

\[
\frac{d}{dt} (m\vec{v}) = q(\vec{E} + \vec{v} \times \vec{B})
\]

Velocity update

\[
\vec{r}_{n+1/2}^{n+1/2} = \vec{r}_{n+1/2}^{n} + q\Delta t \left( \vec{E}_{n+1/2}^{n} + \vec{v}_{n+1}^{n} \times \vec{B}_{n+1/2}^{n} \right)
\]

Leap Frog Scheme

Position update

\[
\vec{r}_{n+3/2}^{n+3/2} = \vec{r}_{n+1/2}^{n+1/2} + \Delta t \vec{v}_{n+1}^{n+1}
\]
Gun Iteration - Space Charge Effect

**Gun Iteration**

1. START
2. Calculate electrostatic field distribution
3. Track particles and monitor space-charge
4. Has space-charge converged?
   - Yes: Go to relaxation of space-charge
   - No: Go to calculate electrostatic field distribution
5. END

Without gun iteration:

With gun iteration:
Tracking Solver - Typical Application (I)

- Cathode
- Focussing electrode
- Anode
- Iron yoke (non linear)
- Permanent magnets

Electron Gun

E-static field

M-static field
Space charge effect is included via gun iteration and space charge limited emission.
<table>
<thead>
<tr>
<th>Feature</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tracking</td>
<td>Solver for particles in static fields including space charge or in harmonic fields excluding space charge.</td>
</tr>
<tr>
<td>Particle In Cell</td>
<td>Self-consistent transient field and particle solver including full space charge effects at all frequencies.</td>
</tr>
<tr>
<td>Wakefield</td>
<td>Transient solver with special beam excitation (predefined fixed straight beam path)</td>
</tr>
</tbody>
</table>
Particle in Cell (PIC) Algorithm

Self-consistent modeling of a collision free plasma.

Macro charges (e.g. $q=10^6$ e\textsuperscript{-})

Relativistic equation of motion

$$\frac{d}{dt}(m\vec{v}) = q(\vec{E} + \vec{v} \times \vec{B})$$

$$\frac{d\vec{r}}{dt} = \vec{v}$$

Current caused by particle motion acts as source in Maxwell’s equations.

$$\text{curl } \vec{H} = \frac{\partial\vec{D}}{\partial t} + \vec{J}; \quad \text{div } \vec{J} = -\frac{\partial \rho}{\partial t}$$

A priori charge conserving algorithm.
PIC Solver - Typical Applications (I)

- Particle Trajectory
- E-Field
- Waveguide Output Power
- Time signal
- DFT

Normalized Spectrum Magnitude

Time Signals

Frequency / GHz
PIC Solver - Typical Applications (II)

[1] Design, simulation and measurement conducted by M. Ruf, K. Thurn and L.-P. Schmidt at Chair for High Frequency Technology, University of Erlangen-Nuremberg
PIC Solver - Typical Applications (III)

## CST PARTICLE STUDIO

<table>
<thead>
<tr>
<th>Module</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Tracking</strong></td>
<td>Solver for particles in static fields including space charge or in harmonic fields excluding space charge.</td>
</tr>
<tr>
<td><strong>Particle In Cell</strong></td>
<td>Self-consistent transient field and particle solver including full space charge effects at all frequencies.</td>
</tr>
<tr>
<td><strong>Wakefield</strong></td>
<td>Transient solver with special beam excitation (predefined fixed straight beam path)</td>
</tr>
</tbody>
</table>
## Wakefield Solver

The Wakefield solver computes the wake potential:

$$
\tilde{W}(x, y, s) = \frac{1}{q_1} \int_{-\infty}^{\infty} \left( \tilde{E}(x, y, z, t = \frac{s + z}{v}) + \tilde{v} \times \tilde{B}(x, y, z, t = \frac{s + z}{v}) \right) dz
$$

- **Excitation (pencil beam with longitudinal Gaussian shape)**
- **Beam path**
- **Integration path**
Wakefield Solver - Typical Application

Beam Position Monitor

Note: Beta smaller than 1 is possible.
New Features Overview
Geometry Handling - Hexahedral Mesh

- CST has extended the numerical algorithms with enhanced material approximation techniques.

**PBA (Perfect Boundary Approximation):**
- Very accurate, but relies on valid CAD shapes.

**FPBA (Fast PBA):**
- Faster than PBA
- Can handle even CAD models with artifacts
- Less accurate as compared to PBA
Geometry Handling - Hexahedral Mesh

EFPBA is now the default algorithm used for solvers based on hexahedral meshes.

Enhanced FPBA provides both the robustness of FPBA and the accuracy of PBA.
Eigenmode Solver

- **Curved tetrahedral mesh** available (up to 3rd order)
- Improved performance and convergence for many examples

Model courtesy of Lancaster University, Dr. Graeme Burt

- Tetrahedral mesh: quick convergence, < 2 min to calculate 9 modes
Eigenmode Solver: Lorentz Force Detuning
Mechanics: Lorentz Force Detuning

Cavity is fixed here
Deformed Mesh (scaled)

Outlook

- Sensitivity analysis for eigenmode solver to evaluate from Lorentz force.
- Automation with System Assembly and Modeling (SAM) possible.
2D Magnetostatic Solver

- Rotational and translational symmetry is available.
- Can be selected in mesh dialog.
- Automatic mesh adaption.
PIC Solver: GPU Computing

Nvidia Tesla 20 cards are supported

Number of Mesh Cells | 1,000,188
Av. Particle Number | 7.74e5
Time CPU (Dual Xeon 5620) | 1h 14m 44s
Time GPU | 12m 25s
Total Speed Up* | 6.02
Time Domain Speed Up | 6.65

* Matrix calculation & post-processing are not running on GPU
PIC Solver: Secondary Electron Emission Models

New model: Vaughan

Advantages:
- Only a few parameters to configure

Disadvantage:
- Limited curve shapes
- Only true secondaries
- Not supported on the GPU, yet.
New model: Import

Advantages:
- Easiest definition
- Loading of measurement data possible
- GPU support

Disadvantage:
- Only true secondaries
Post Processing - Emittance

Emittance definition used:

$$\epsilon_{x,rms} = \sqrt{\langle x^2 \rangle \langle x'^2 \rangle - \langle xx' \rangle^2}$$

Emittance often used by accelerator people:

$$\epsilon_{n,rms} = \beta \gamma \epsilon_{rms}$$
Any Questions?