Emission Modeling for PITZ

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Introduction

- Large differences are found between measurement and simulation - optimum emittance vs. spot size, spch limit, …
- Find source of discrepancy on simulation side

M. Krasilnikov, FEL 2013
Introduction

- Hypothesis 1: problems originate at the cathode / gun
- Hypothesis 2: beam dynamics at emission time not properly modeled

Particle velocities at emission time

Inertial frame codes (Astra, Parmela, …)
- Relative particle motion neglected
- Retardation effects (partially) omitted
- No acceleration radiation

Full EM simulations
- Particle-Particle (PP) codes
- Particle-In-Cell (PIC) codes
Introduction

- Lienard-Wiechert PP

\[ E = \frac{q}{4\pi\varepsilon_0} \left[ \frac{(n - \beta)(1 - |\beta|^2)}{(1 - \beta \cdot n)^3 R^2} + \frac{n \times (n - \beta) \times \beta}{(1 - \beta \cdot n)^3 R} \right] \]

- Store full history of trajectories
- Search retarded interaction point for every particle-particle pair
- Scaling: \( N^2 \times \Delta t^2 \)
Introduction

- Discontinuous Galerkin (DG) PIC

FEM-like field approximation on grid with high order basis functions

Weak form of Ampere's law

\[ \int d^3r \frac{\partial \bar{E}}{\partial t} \varphi - \int d^2r (n \times F_H) \varphi + \int d^3r (\nabla \varphi) \times \bar{H} = 0 \]

Numerical interface fluxes

\[ n \times F_E = \frac{1}{2} n \times [\bar{E}(r^-, t) + \bar{E}(r^+, t)] \]

\[ n \times F_H = \frac{1}{2} n \times [\bar{H}(r^-, t) + \bar{H}(r^+, t)] \]
Introduction

- Discontinuous Galerkin (DG) PIC

Current density approximation

\[ \mathbf{j}(\mathbf{r}, t) = \sum_{p} Q_p \mathbf{v}_p(t) W_p \left[ \mathbf{r} - \mathbf{r}_p(t) \right] \]

Grid projection

\[ \mathbf{j}_i^e (t) = \sum_{p} Q_p \mathbf{v}_p(t) \int_{\Omega_{ep}(t)} d^3 \mathbf{r} W_p (\mathbf{r}, t) \varphi_i^e (\mathbf{r}) \]

Total grid current / time step

\[ \mathbf{J}_i^e (t^n, t^{n+1}) = \int_{t^n}^{t^{n+1}} dt \mathbf{j}_i^e (t) \]
SPCH Simulations in the Gun

- Beam dynamics over short distance (up to 2cm behind cathode)
  - Sufficient to observe possible issues at emission time
  - Analyze numerical convergence
  - Identify numerical parameters for full-scale simulations
  - Perform comparison between different approaches
  - Estimate space charge limits

- 3D-simulations throughout the following (except for Astra)
  - Nom. parameters/ PITZ-1.8: Q = 1nC, FWHM: 20/2 ps, XY_rms = 0.4mm, …
SPCH Simulations in the Gun

- LW-PP convergence

wrt. time step

wrt. number of particles
SPCH Simulations in the Gun

- DG-PIC convergence

wrt. approximation order

wrt. number of particles
SPCH Simulations in the Gun

- CST PS (PIC) convergence

finest mesh resolution

relative error for the best two mesh resolutions
SPCH Simulations in the Gun

- CST PS (PIC) performance

![Graph showing CPU time vs. mesh cell numbers]

**Calculation Domain in CST:** z = (0-3) cm
Photocathode @ z=0

**Computer Configuration Info:**
- CPU: 2 * Intel Xeon E5-2643 (Quadcore, 3.30 GHz, 2 * 8.0 GT/s, QPI, 10 MB L2 Cache)
- Memory: 256 GB
- Harddisk: 500 GB SATA RAID1 + 3000 GB

**Finest Mesh Resolution**
\[ \Delta x \approx \Delta y \approx \Delta z \approx 0.01\text{mm} \]

- Calculation domain in z direction = 3cm
- Calculation Time = 29 hours
- Meshcell Numbers = 1095 Millions
SPCH Simulations in the Gun

- CST PS (PIC) performance

**Computer Configuration Info:**

- CPU: 2 x Intel Xeon E5-2643 (Quadcore, 3.30 GHz, 2 x 8.0 GT/s QPI, 10 MB L2 Cache)
- Memory: 256 GB
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**Finest Mesh Resolution**

- $\Delta x \approx \Delta y \approx \Delta z \approx 0.01 \text{mm}$

**Calculation domain in $z = 3\text{cm}$**

- Meshcell Numbers $\approx 1095\text{millions}$
- Peak Memory Needed $\approx 254 \text{GB}$
SPCH Simulations in the Gun

- Comparison

(full EM vs. inertial frame)
SPCH Simulations in the Gun

- Comparison

slice emittance (@ 2cm)

slice energy spread (@ 2cm)
SPCH Simulations in the Gun

- Comparison for other bunches (Q = 1nC)

\[ XY_{\text{rms}} = 0.5\text{mm} \]

\[ XY_{\text{rms}} = 0.6\text{mm} \]
SPCH Simulations in the Gun

- Origin of discrepancy

\[
E = \frac{q}{4\pi\varepsilon_0} \left[ \frac{(n - \beta)(1 - |\beta|^2)}{(\beta \cdot n)^3 R^2} + \frac{n \times (n - \beta) \times \dot{\beta}}{(\beta \cdot n)^3 R} \right]_{t=t_r}, \quad B = \frac{1}{c} \frac{n \times E}{t=t_r}
\]

single particle fields

<table>
<thead>
<tr>
<th>Hierarchy of approximations</th>
<th>retardation</th>
<th>contraction</th>
<th>radiation</th>
<th>relative motion</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \beta = 0 )</td>
<td>E-statics (ES)</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>( \beta^2 \ll 1 )</td>
<td>E-statics / B-statics (ES-MS)</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>( \beta = \text{const.} )</td>
<td>bunch in uniform motion / average frame (UMAF)</td>
<td>‡</td>
<td>‡</td>
<td>–</td>
</tr>
<tr>
<td>( \frac{\partial \beta}{\partial t} = 0 )</td>
<td>individual particles in uniform motion / local frame (UMLF)</td>
<td>‡</td>
<td>‡</td>
<td>–</td>
</tr>
</tbody>
</table>

SPCH Simulations in the Gun

- Origin of discrepancy
Emittance at EMSY1

XY_rms = 0.4mm
Emittance at EMSY1

- $XY_{\text{rms}} = 0.4\text{mm}$
- $XY_{\text{rms}} = 0.5\text{mm}$
- $XY_{\text{rms}} = 0.6\text{mm}$
Emittance at EMSY1

- spch limit @ > 0.4mm
- spch limit @ > 0.25mm

- Same "optimal" XY_rms

- 2nC
- 1nC
- 0.1nC
Emittance at EMSY1

Astra
1nC
XY\_rms = 0.4mm

DG-PIC
1nC
XY\_rms = 0.4mm
Emittance at EMSY1

DG-PIC
1nC
XY_rms = 0.35mm

DG-PIC
1nC
XY_rms = 0.3mm
Transverse Spot Inhomogeneities

Laser

QE map

Charge density

Cath_11.3
XY_rms = 0.3mm

Cath_110.2
XY_rms = 0.3mm
Transverse Spot Inhomogeneities

- Emittances up to 7cm

Particles go lost at the cathode.
Space Charge Limits

Charge extraction – $Q_{\text{bunch}} = 1\text{nC}$

- $Q_{\text{XY}} \approx 0.3\text{mm}
- Q_{\text{bunch}} \approx 0.9\text{nC}
- Q_{\text{bunch}} \approx 0.75\text{nC}$
Space Charge Limits

Charge extraction – $Q_{\text{bunch}} = 1\text{nC}$

numerical convergence?

$XY_{\text{rms}} = 0.25\text{mm}$

~$0.9\text{nC}$

~$0.75\text{nC}$
Space Charge Limits

Charge extraction – $Q_{\text{bunch}} = 1\text{nC}$

DG convergence
$XY_{\text{rms}} = 0.3\text{ mm}$
Space Charge Limits

Charge extraction – $Q_{\text{bunch}} = 1 \text{nC}$

DG (non-) convergence
$XY_{\text{rms}} = 0.25 \text{ mm}$
Space Charge Limits

Charge extraction – $Q_{\text{bunch}} = 1\text{nC}$

CST PS (non-) convergence
Space Charge Limits

Charge extraction vs Q_bunch

Used assumption on source limited emission is probably wrong (?)

Q (nC)

z (mm)

-50  -40  -30  -20  -10   0    10   20   30   40   50

0     0.2   0.4   0.6   0.8   1.0  1.2  1.4  1.6  1.8

measured charge, XYrms=0.3mm, LT=62%
measured charge, XYrms=0.3mm, LT=100%
simulated charge, XYrms=0.3mm, Q=1 nC
simulated charge, XYrms=0.4mm, Q=1 nC

PP: 10nC - 50k / 50fs - 5um
PP: 10nC - 100k / 50fs - 5um
PP: 5nC - 100k / 50fs - 5um
PP: 5nC - 200k / 50fs - 1um
PP: 5nC - 500k / 50fs - 1um
DG: 5nC - 500k / 50fs - 10um
Conclusions

- Modeling errors exist in Astra simulations
  - charge expansion effects at the cathode are neglected
  - projected emittance is overestimated: ~20% off at 1nC / 0.4mm
  - Predicted SPCH limits are lower than should be if source limited emission is assumed

- But, systematic shift in the optimal parameters (spot size) cannot be explained by these “numerical problems”

- The emission regime is yet unclear
  - If spch limitation occurs (partially) completely different beam dynamics is to be expected

@5pC
Thank you for your attention