Delayed Photo-Emission Model For PIC Codes

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Photocathode Physics for Photoinjectors (P3)

Theory and Simulation

Sections Outline

Outline

GOALS

- Development of physics- and materials-based time-delayed photoemission model that captures sub-micron features
- Models to enable the prediction of emittance, quantum efficiency (QE) and dark current from microscale structures with nanoscale features

Background:

- High QE photocathodes = semiconductors: contain Cs to reduce emission barrier.
- A fraction of e^- that escape undergo collisions prior to emission, but standard beam optics code models neglect their contribution.
- x-Ray FEL's: pulse lengths $\lesssim 1$ ps $\leftrightarrow$ scattered e^- cause tail to emission bunch, interacts poorly with space charge, increases $\varepsilon_{n,rms}$ $\leftrightarrow$ halo (e^- outside core beam).

1. Describe time-dependent model of emission accounting for material properties, scattering mechanisms, surface barriers, laser interaction parameters, and time & energy dependence of the delayed emission.
2. Discuss incorporation of these models into Particle-in-Cell code MICHELLE to address pulse elongation and emittance effects due to photocathode

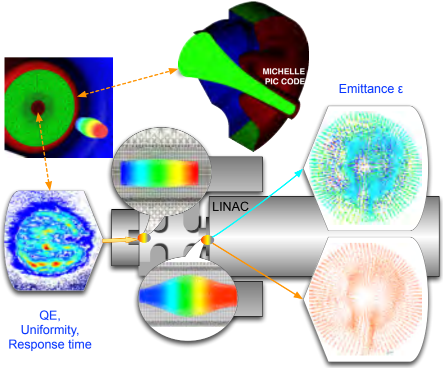
Future x-Ray Sources & Colliders

The Need

Future Coherent x-Ray Sources & Advanced Colliders address need for sustainable energy, scaling of computational power, detection / mitigation of pathogens, study of structure & dynamics of cells

The Problem:

- To access, observe, control matter on timescale of electronic motion and spatial scale of atomic bonds, high performance e^- beams are demanded.
- Performance requirements exceed state-of-the-art for lifetime, QE, $\varepsilon_{n,rms}$. These requirements are related to emission uniformity and response time.
- Modeling effects needed for design but existing emission models do not account for emission delay, surface profilimetry.



Energy Spread and Delayed Emission

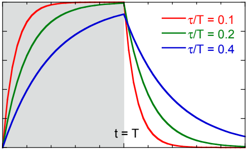
A simple model of delayed emission: flat-top pulse $I_\lambda(t)$ of width T defined by ($\Theta(x)$ is Heaviside step func.)

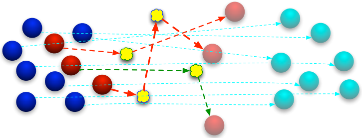
$$I_\lambda(t) = I_o \Theta(t)\Theta(T-t) \qquad (1)$$

Then if emission is delayed by a factor τ, the emitted current $I_e(t)$ is

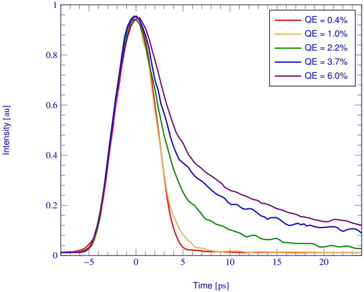
$$I_e(t) = \frac{QE}{\tau}\int_{-\infty}^{t} I_\lambda(s) e^{-(t-s)/\tau} ds \qquad (2)$$

$$\propto \begin{cases} 1 - e^{-t/\tau} & (t < T) \\ \left(e^{T/\tau} - 1\right) e^{-t/\tau} & (t > T) \end{cases} \qquad (3)$$





Scattering: creates a population of lower energy e^- that fall behind ballistic e^-, contributes to E spread

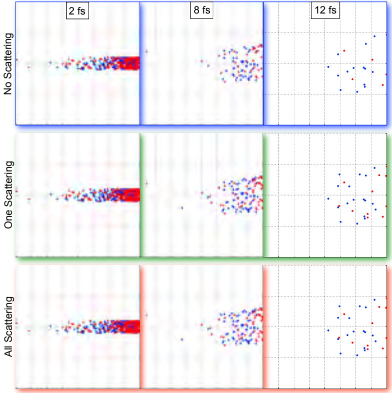


Ddelayed emission from GaAsP after Fig. 9, of I. Bazarov, et al., PRSTAB11, 040702 2008. Observe diffusive tail!

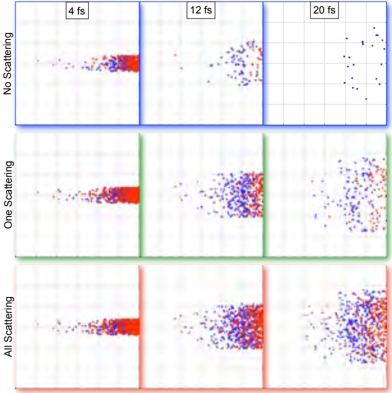
Response Time and Scattering

Monte Carlo. 1000 e^-. Surface is right hand boundary, incident laser is from the right
Top: Fatal approximation; Middle: one scattering; Bottom: all electrons such that $E > \mu + \phi$

Figures from: Jensen, *et al.*, J. Appl. Phys., **110**, 034504 (2011).



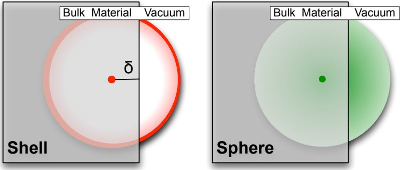
Bare Cu : $\Delta t = 6$ fs, $t_o = 2$ fs. When $E < \mu + \phi$, electron is removed from simulation. Length of simulation region $= 12$ nm. Fatal approximation is reasonable.

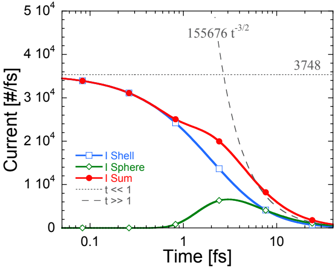


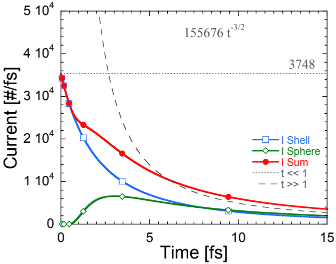
Cs on Cu : $\Delta t = 8$ fs, $t_o = 4$ fs. Scattered electrons may be emitted if $E > \mu + \phi$. Length of simulation region $= 16$ nm. Fatal approximation neglects too much.

Sections Outline

Simple Model: Shell and Sphere







- Shell: Expanding rim of charge and unscattered electrons
- Sphere: Expanding cloud of charge and thermalized electrons
- All e^- photoexcited at depth δ; Monte Carlo simulation
- Charge through surface = sum of Shell & Sphere: $I(t) = dQ/dt$

$$I(t) = Q_s \frac{t_o}{2(t+t_o)^2} + Q_d \left(\frac{\tau *}{4\pi t^3}\right)^{1/2} \exp\left(-\frac{\tau *}{t}\right) \quad (4)$$

Q_s and Q_d are total charge in either shell or sphere; t_o and τ^* are fitting parameters (latter related to relaxation time) determined by Monte Carlo.

Multiple Shells in Constant Field

- Multiple Shells dQ expand as per Eq. (4); $\Delta Q(t)$: sum over shells
  - Charge per shell: $dQ \propto \exp(-x/\delta)\,\Delta x/\delta$ where x = distance into bulk and Δx = width of shell.
  - Current $\Delta I(t) = d\Delta Q/dt$
  - Field at surface held constant; Diffusion model unchanged.
- Shell Integration = total current from unscattered e^-:

$$I_{shell}(t) = Q_{shell}\frac{v_o e^{-s_o}}{2\delta s_o^2}\left\{(e^s - 1)(1 + s_o) - se^s\right\} \quad (5)$$

$$v_o = \left(\frac{2(\hbar\omega + \mu)}{rm_o}\right)^{1/2} \quad s_o = \frac{v_o t}{\delta}; \quad s = s_o\left[1 - \left(\frac{\phi + \mu}{\hbar\omega + \mu}\right)^{1/2}\right]$$

- Due to photo-excitations near the surface, current emitted immediately but exponentially declines in time
- Ripples & noise on laser pulse smoothed by convolution of photo-excitations distributed over length.

$F = q\mathcal{E}$ = surface field

$Q = 0.36$ eV-nm $\rightarrow$ image

μ = Fermi level

Φ = work function

v_o = velocity

δ = laser penetration depth

$\phi = \Phi - \sqrt{4QF} \rightarrow$ Schottky

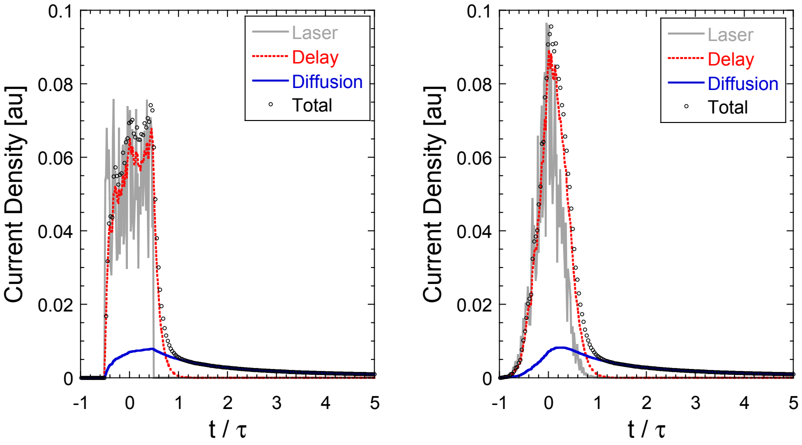
$\hbar\omega$ = photon energy

$r = m/m_o$

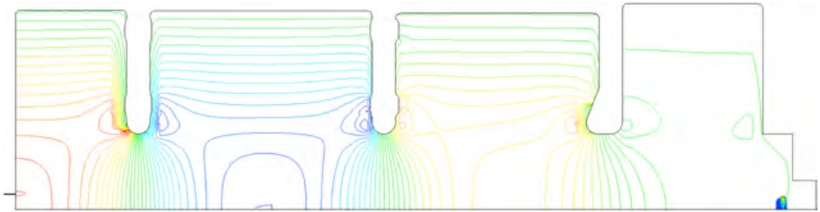
m_o = rest mass.

Laser Jitter: Cu-like

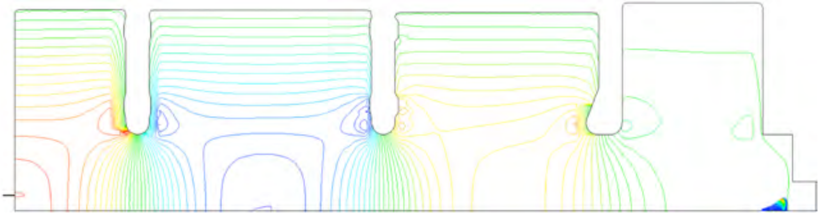
(Left) Flat-top; (Right) Gaussian
Observe amount of charge in tail!



RF Gun Sim: Non-Delayed Vs. Delayed

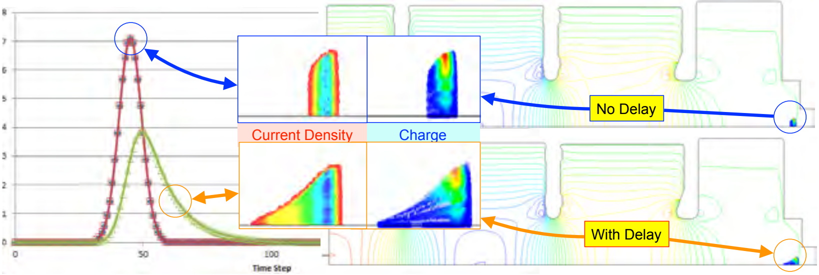


Non Delayed-Emission model results - no field or secondary emission. One emission pulse.



Delayed-Emission model results - no field or secondary emission. One emission pulse.

RF Gun Sim: Pulse Shape Comparison



Three delay mechanisms shown in Graph of Intensity vs. Time Step:

- Blue: no delay (follows laser pulse; under red line).
- Red: delay equal to one time step (shows integrated quantities dealt with properly on the sub-time-step scale).
- Green: delay span (tail) of ≈ 5 FWHM of the laser pulse.

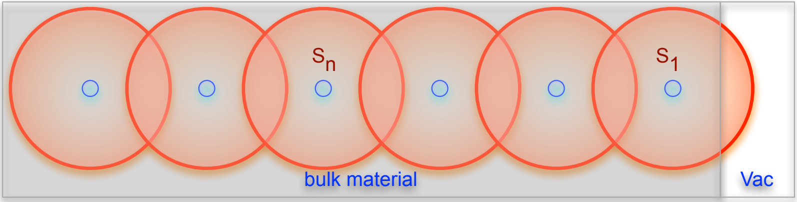
The charge density shows how the delayed emission affects both the charge distribution as well as the shape of the pulse. The tail of the beam gets compressed radially in both cases, however the non-instantaneous nature of the emission delay can be seen to affect the timing of the pulse, and this would have to be compensated for in a real device.

Next Generation Model

Modify Moments Approach for field $F(t)$ and Materials Physics inclusions. The quasi-steady state formulation ($T \gg \tau$ or $\delta/(\hbar k_F/m)$) is represented as a three-step process of Emission + Transport + Absorption

$$M_n(k_j) = \frac{1}{(2\pi)^3} \int d\vec{k} \left[k_j^n\right] [\mathrm{E}] [\mathrm{T}] [\mathrm{A}] \leftrightarrow QE = \frac{(1-R)M_1(k_z)}{2M_1(k)|_{D=f_\lambda=1}} \quad (6)$$

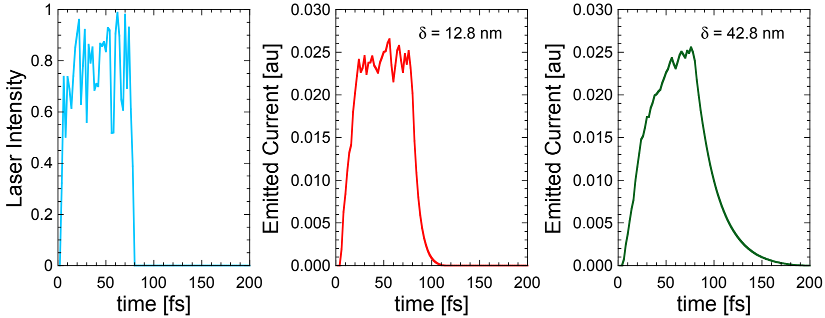
Transport module now replaced by an Expanding Sphere Model



Shells located on lattice of points s_n (blue: initial; red: after time t). Emission naturally time-delayed by time-of-flight from s_n to surface. Emission into vacuum governed by field that exists *at surface when shell crosses it* and is therefore inherently time-dependent. Q = charge in vacuum: $I = dQ/dt$

Response Time and Pulse Shape

$Q(t)$ (charge in vacuum) is governed by: Laser penetration depth $\delta(\omega)$; velocity of expanding shell $\approx \hbar k_F/2m$; and time dependence of emission probability. Current density therefore depends on them as well.

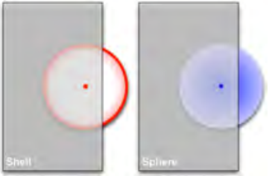


Effects of different penetration depth $\delta(\omega)$: Ad hoc laser jitter (noise) = 50%. $\Phi = 2.1$ eV. Laser pulse set to 80 fs top-hat, plus 50% jitter. Barrier height set to $\mu + \Phi - \sqrt{4QF(t)}$. Surface field is time-dependent: $F(t = t_j) = F_o(N_t + j - 2)/(N_t - 1)$ with $F_o = 100$ eV/μm (linearly increasing)

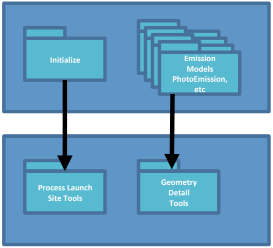
Sections Outline

STTR SOLUTION

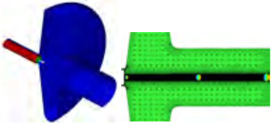
- Develop new physics-based emission models for application to high quantum efficiency photocathodes



- Implement these models into a portable library that can be incorporated to a wide range of existing code types



- Incorporate library into the particle-in-cell (PIC) MICHELLE and the meshless MICHELLE-eBEAM beam optics codes



Develop New Physics-Based Emission Models

Physics-Based Emission Model Development:

- Develop the first generation delayed emission models: These models will be physics based and developed into mathematical solutions and algorithms and tested separately before implementation into the beam optics codes.

Three technical approaches to be undertaken, all refer to modeling associated with photoemission and field emission near the surface. They are:

1. The first generation delayed emission models
   Prompt (shell) and delayed (sphere) emission models for multiple sites as a function of material parameters
2. Sub-micron surface roughness and dark current models
   Point charge and line charge models; impulse trajectory model; space charge effects
3. Interaction of delay and roughness via space charge using transit time and trajectory modeling approaches

Explanation

- Delayed emission models for planar surface are primary: incorporation into MICHELLE environment is Phase I
- Surface roughness models require theory/code to handle Point and Line Charge models and relation to transit time approach: Phase II
- Space charge transit time available for planar surface case, but require code development for 2D and 3D configurations; begin in Phase I, majority in Phase II

Implement Models Into Portable Library

Design the emission software architecture that supports

- The emission model development through both phases of the STTR
- Existing emission models and models that are currently under development
- Future needs to accurately represent the emission physics

Develop new emission software library prototype

- Develop the emission software architecture prototype that contains the current emission models as well as the new delayed emission model

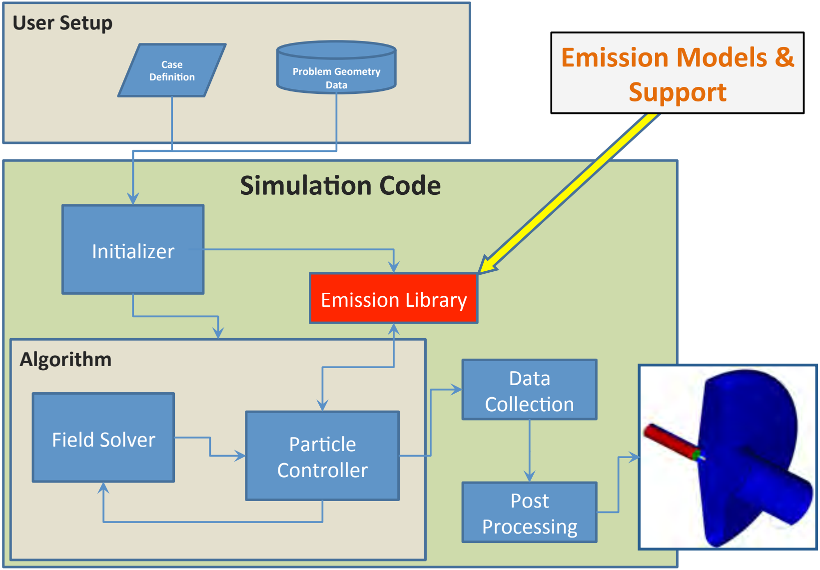
Implement first generation delay model into the MICHELLE Toolset

- Employ the new emission software library prototype
- Implement the first generation into the MICHELLE PIC code. The architecture will be completely new and designed to supplant that already in MICHELLE
- Test the library in MICHELLE

Test and validate

- Test the implementation against the theoretical model for consistency

Typical Beam Device Simulation Architecture



Model Simulation Case Component "Ownership"

Host Code only

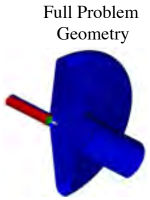
- Geometry

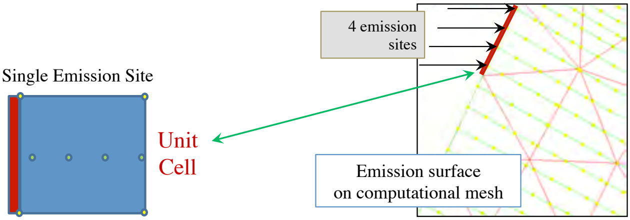
Both Host Code and Emission Library

- Material properties (Initialization)
- Surface finish (Initialization)
- Fields (Every time step)
- Temperature (Every time step)

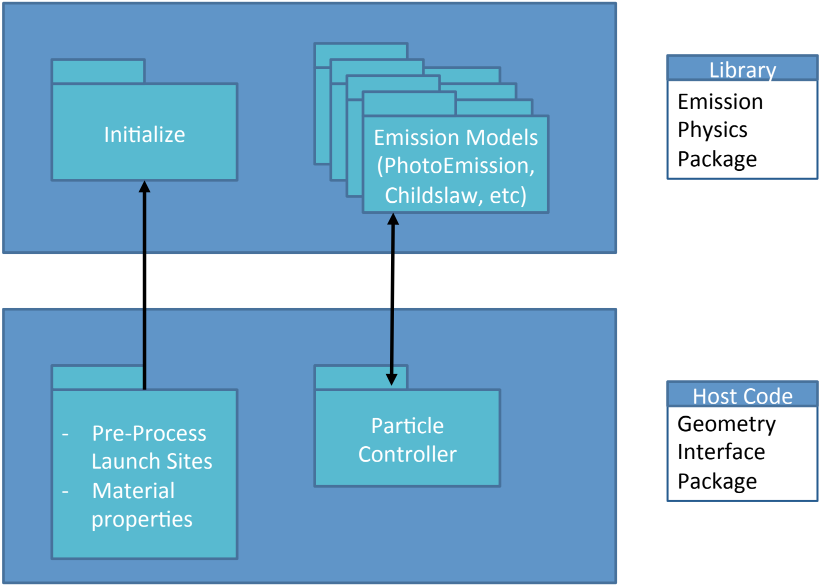
Emission Library

- Operates at the unit cell level
- One unit cell ↔ One emission site

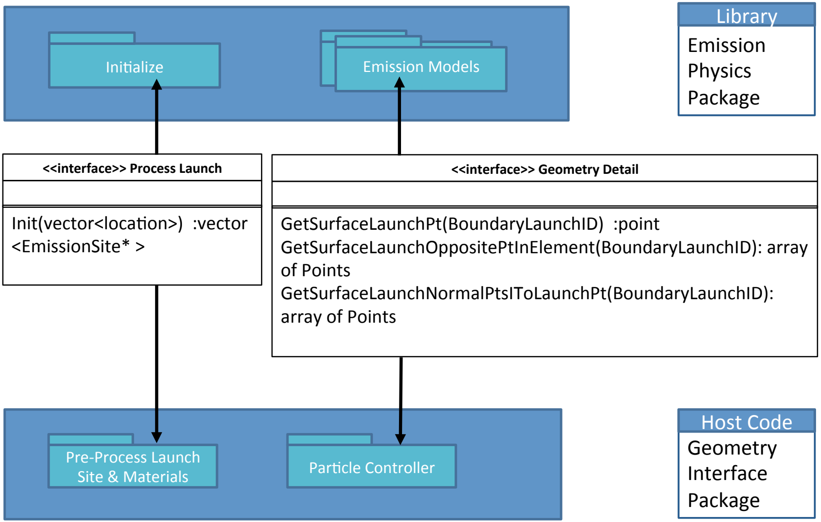




Package Diagram of Functional and Static Setup Layers



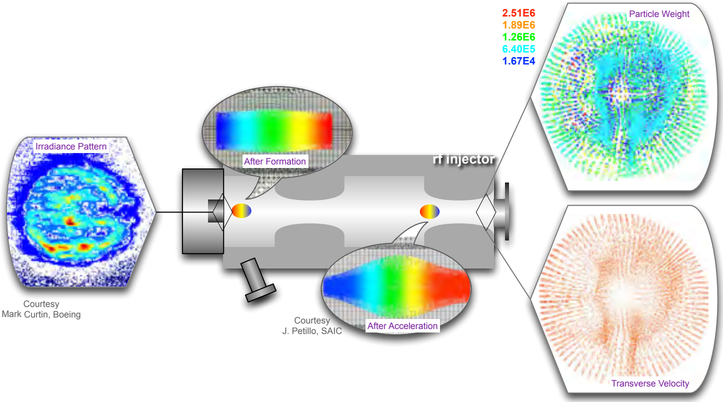
Interface Diagram of Layer Interaction Calls by Package



Photoemission Models in Beam Code

SIMULATION: How spatial irradiance pattern affects Beam quality created from photoemission process

- Photoemission model implemented into NRL/SAIC MICHELLE code: model applied to AES/BNL SRF Gun
- Simulation results confirmed PARMELA-B calcs for gross parameters like emittance and RMS beam size
- model can be used to investigate more detailed beam formation in gun:
  - will confirm in what parameter range PARMELA-B results can be used
  - gives insight into internal beam dynamics of bunch
- Implementing and testing Field Emission model and Predict Dark Current

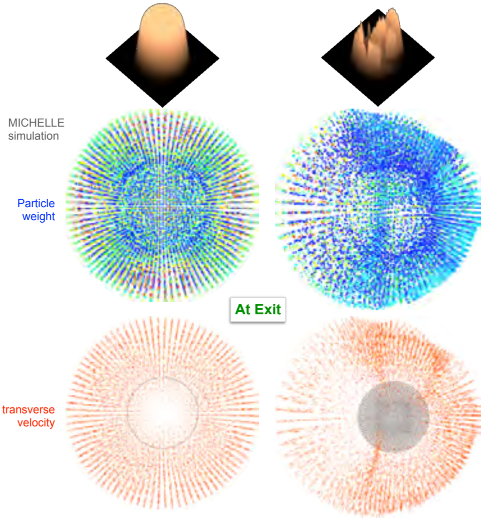


Courtesy
Mark Curtin, Boeing

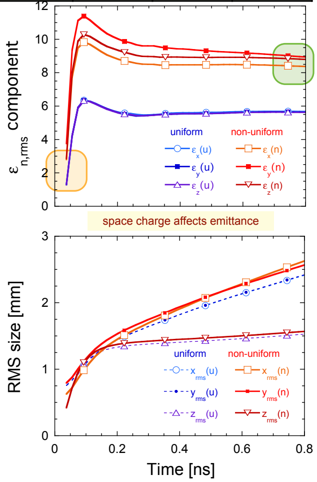
Courtesy
J. Petillo, SAIC

Non-Uniformity and Emittance Growth

Looking down the bunch:



% Change	ε-x	ε-y	ε-z
Initial	116%	190%	120%
final	47%	59%	56%



PIC Code Implementation

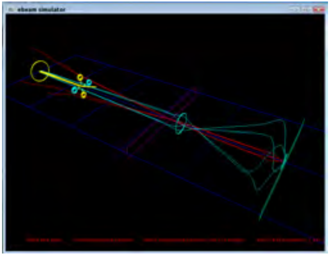
Library Approach

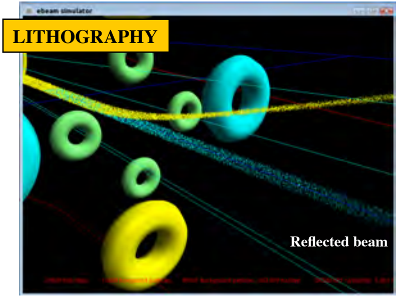
- A library is under development to house the software to make is accessible by other codes
- The library will be written to support multithreading and GPU processors
- The library is not simply emission models, but a more substantive framework allowing it to provide utility functions including
  - Laser temporal profiles
  - Laser spatial profiles and gating
  - Laser jitter & spatial irradiance fluxuation
  - Thermal Field Emission in addition to the Photoemission discussed

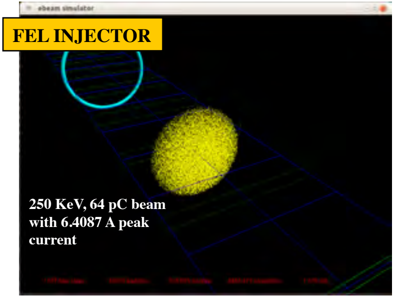
MICHELLE eBEAM: Meshless Beam Optics Code

Meshless electrostatic beam optics code

- Heterogeneous CPU/GPU/TBB - developed since 2007
- Coulomb interactions on GPU
  - Direct n^2 and tree-code $n \log(n)$ algorithms
  - Counter Streaming beams with scattering
- High accuracy particle integration - Up to 8^{th} order
- Performance: Fully 3D GPU as fast as a 2D CPU code

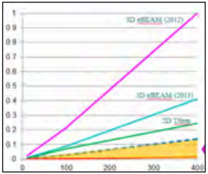






MICHELLE *e*BEAM (I)

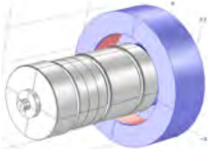
- Mesh-based FEL beamline codes spatial resolution is limited to its cell size
  - The smallest scale that can be resolved is often much larger than the particle spacing
  - 2D is reasonably fast, but 3D is not
- Mesh-less approaches do not have such a limitation / Coulomb calculations are preferred GPUs have shown the ability to efficiently handle the n-body, like Coulomb, gravitational, etc.
- Demonstrated that the GPU solution is viable and provides a performance advantage
  - 3D calculation for the price of 2D
- Proven that eBEAM can handle beamlines typical of MW-grade FELs
  - New prototyped physics models (Self-B, Photoemission, Image charge, 1D CSR)
  - Prototyped extensions to handle high bunch charge beamlets (macroparticles, DC & RF field maps, I/O)

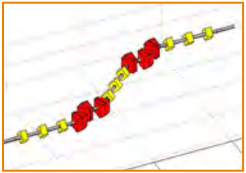


- What distinguishes the new code from todays FEL codes? (Comparing to codes like PARMELA, TStep, Elegant, GPT, and DIMAD)
  - Mesh-less: resolution only limited by the number of particles
  - Has the ability to process large particle counts, capturing the effects of higher order particle effects
  - Captures detailed physics with performance that will allow optimization searches and S2E modeling
  - Capability allows beamlet tails and beam halo to be modeled, uncovering performance degraders
  - Is fast: Performance that can be instrumental to the commissioning of components and systems

MICHELLE *e*BEAM (III)

- Photo-Injector simulation requirements:
  Photoemission, field emission, thermal field emission & secondary emission models, RF drive fields, applied fields, field maps, robust self field models
- RF boosters ERL simulation requirements
  RF drive fields, applied fields, field maps
- Magnetic transport section simulations, including merges & transport lattices, bunchers
  Applied fields, field maps, CSR
- General simulation requirements
  Import/export of particle and field data (support of S2E)
  Supporting compatible IO data structures between community codes
- MICHELLE vs. MICHELLE-eBEAM
  - MICHELLE Proper: Single beamline component modeling
  - MICHELLE-eBEAM: Multiple beamline component modeling





Summary

First Generation Delayed Emission Model

- Demonstration of 1^{st}-Gen (constant surface field) Delayed Photoemission model: shell model for unscattered e^- and diffusion model for scattered e^-.
- Incorporated 1^{st}-Gen model into Particle-in-cell code MICHELLE.
- Examined impact of delayed emission in PIC simulation of Photoinjector gun.

Next Generation Delayed Emission Model

- Time-dependent emission model developed for changing surface field $F(t)$
- Ability to treat few-scattered electron contributions enabled.
- In Progress:
  - Incorporation of material properties $(m, E_G, n$ & $k, R, \delta, DOS)$ for metal, semiconductor, and coated material photocathodes
  - Geometry / Field enhancement modeled using an impulse approximation to the launch velocity of electrons