Lecture 10: Injector Simulations

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Why simulations?

Photoinjector systems are complex environments with many external and internal forces acting on an initial beam distribution.

It is not possible to obtain by analysis a complete description of the motion of $\sim 10^9$ - 10^{10} electrons that includes all of their interactions with each other and the beamline elements.

•We perform simulations to better approximate the real world conditions

- Complex particle distributions
- Non-analytic forces and interactions

•We perform simulations to increase our knowledge of the behavior of these systems

- Benchmark analytic estimates and find ranges of validity
- Benchmark measurements and find sources of experimental errors
- Explore areas of relative uncertainty



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What can we simulate?

Photoinjectors are largely governed by the rules of classical mechanics, electrodynamics, plasma physics, and special relativity. We have simple rules to apply that govern the motion of charged particles in fields.

The role of a photoinjector is to generate a bunch of electrons, and to manipulate them and transport them to another accelerator system for eventual use in creating high brightness beams of electromagnetic radiation, to use in medical diagnostic and treatment, or to study particle interactions at the nuclear and sub-nuclear levels.

Our primary interest is in determining how the 6D distribution of beam particles evolves from generation to eventual extraction.

We may also be interested in how the beam-generated fields interact with the environment.



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What is difficult to answer with simulations?

Simulation is a branch of *phenomenology*, in that it seeks to connect various empirically observed phenomena in way that is consistent with theory, but is not direct derivable from theory.

As such, we can not hope to answer with simulations those questions that go beyond the range of validity of the underlying theories provide the rules by which the simulation operates.

Our model of beam dynamics depends on a *classical* description that is derived from the *collisionless Vlasov-Boltzmann equation*. It is a *kinetic* description that tracks particles and distributions. It does not attempt to describe *stochastic* phenomena. Our model does not contain any description of *quantum mechanics*, so all behavior is strictly deterministic. Any uncertainties arise due our incomplete knowledge of the environment or initial conditions.



Defining the model

One of the first tasks is to define our model.

What are the important questions we seek to answer? What is the relevant geometry to describe the fields and motions? What elements are necessary to explore the relevant phenomena?

Once we know the purpose to our study, we can more easily describe the scope of the simulation and the needed resources.

- How much can we utilize prior analytic or numerical results/methodology?Will a 1D or 2D geometry suffice, or do 3D effects need to be considered?Will time-dependent fields be necessary, or can we static or quasi-static descriptions?
- Do I care about bunch-scale dynamics? Sub-bunch?
- How many particles are necessary to capture the essential physics and phenomena?



RF design codes

- SUPERFISH, HFSS, URMEL, MAFIA/MW Studio, ANSYS, etc. etc.
- Analytical models
 - Pill box cavity, Sinusoidal rf fields, wakes
- Time domain vs. frequency domain
- Eigenmodes
 - 2D, 3D
 - Field distributions, effects due to loss of symmetry
 - Peak fields in structure, surface heating, multipacting sites
- Time dependent fields
 - Multimode effects (pi + zero modes, eg.)
 - Transient to steady state effects (risetime, waveform ripple, etc.)
 - Power coupling studies, rf gymnastics
 - Wakefields







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7 Cell Cavity Benchmarking



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Magnetostatic codes

- POISSON, OPERA/TOSCA/RADIA
 - Essential for 2D,3D problems with arbitrary conductors and permanent magnets.
- Analytical models for simple geometries and currents

Solenoid magnet field

$$B_{z}(r=0,z) = \frac{B_{0}}{1+(z/a)^{2}}$$
 (Reiser, p.177)

Somewhat better fit to experimentally measured profiles is given by Bernal, et. al., Phys. Rev. ST - Accel. Beams 1, 044202 (1998).

$$B_{z}(r=0,z) = B_{0} \exp\left[-\frac{z^{2}}{d^{2}} \left(\sec h \left[\frac{z}{b}\right] + c_{0} \sinh^{2} \left[\frac{z}{b}\right] \right)$$



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Hierarchy of beam simulations

- Single particle
- Slice codes
 - TRACE3-D, HOMDYN
- Multiparticle
 - PARMELA, ASTRA, GPT, Impact-T, elegant
- Self-consistent PIC codes
 - MAFIA/Beam Studio, VORPAL, MAGIC, ...



Single Particle (1st order moments)

In many instances, we may model the behavior of a entire electron beam with a single representative particle. This is helpful in tracking the evolution of the beam as a whole (collective motion).

> Beam energy Time-of-flight Beam trajectory and correction

Phase (time) and energy jitter

This type of simulation can be quite fast.



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RMS (2nd order moments) description

The 2nd order beam moments are useful for

Focusing strengths, magnet tuning, matching beam envelopes Lowest order space charge effects Individual slice and slice-to-slice variations

projected emittance

beam break-up instabilities (multiple bunches)

Beam Matrix

$$\Sigma = \begin{bmatrix} \left\langle x^2 \right\rangle & \left\langle xx' \right\rangle & \left\langle xy \right\rangle & \left\langle xy' \right\rangle & \left\langle xz \right\rangle & \left\langle xz' \right\rangle \\ \left\langle xx' \right\rangle & \left\langle x'^2 \right\rangle & \left\langle x'y \right\rangle & \left\langle x'y' \right\rangle & \left\langle x'z \right\rangle & \left\langle x'z' \right\rangle \\ \left\langle xy \right\rangle & \left\langle x'y \right\rangle & \left\langle y^2 \right\rangle & \left\langle yy' \right\rangle & \left\langle yz \right\rangle & \left\langle yz' \right\rangle \\ \left\langle xy' \right\rangle & \left\langle x'y' \right\rangle & \left\langle yy' \right\rangle & \left\langle y'^2 \right\rangle & \left\langle y'z \right\rangle & \left\langle y'z' \right\rangle \\ \left\langle xz \right\rangle & \left\langle x'z \right\rangle & \left\langle yz \right\rangle & \left\langle y'z \right\rangle & \left\langle z^2 \right\rangle & \left\langle zz' \right\rangle \\ \left[xz' \right] & \left\langle x'z' \right\rangle & \left\langle yz' \right\rangle & \left\langle y'z' \right\rangle & \left\langle zz' \right\rangle & \left\langle z'^2 \right\rangle \end{bmatrix}$$

det Σ is proportional to emittance (2D, 4D, 6D)



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TRACE3-D Model

- K. Crandall, D. Rusthoi (LANL), LA-11054-MS (1987).
- Tracks 6D beam matrix through linear elements.

 $\Box \ \Sigma = \mathsf{M}\Sigma_0\mathsf{M}^{\mathsf{T}}$

- No emission physics.
- Uses linear space charge forces inside uniform ellipsoid no space charge induced emittance growth.
- Fast. Good for tuning beamline focusing properties.



HOMDYN Beam Dynamics Model

- The bunch is a uniformly charged cylinder, segmented into longitudinal slices.
 - Thermal emittance is constant for each slice
 - Incoherent energy spread is neglected.
- Each slice sees particular external (time-dependent) fields, and slice position-dependent self fields.
- Transverse dynamics for each slice is governed by an individual slice envelope equation.
- Longitudinal dynamics for each slice is handled by a single particle equation of motion.
- Fast. Can calculate projected emittance oscillations and growth. Useful for beamline tuning for emittance compensation, and scans over large parameter space regions.



Multiparticle codes

- Produces the most detailed studies, includes the most comprehensive description of physical phenomena
 - uses real particles or macro-particles
- Most computationally expensive to run
 - Increases geometrically with number of dimensions; linearly with particle number, length/duration of simulation
- Susceptible to noise, numerical instabilities, sensitivity to initial conditions in beam distribution
- PARMELA, ASTRA, GPT, Impact-T, VORPAL, elegant
 - Useful to benchmark against experiment.
 - Requires detailed information on initial beam distribution, field profiles and fringe fields, 2D or 3D alignment errors, etc. to accurately model real systems.



Electrostatic self-fields

Typically the most computationally costly sector of multiparticle tracking is in calculating the self-field impulses.

Beam self-fields are calculated in the beam rest frame

Relativistic dilation along longitudinal direction

Difficult to maintain space charge cell aspect ratios, and accuracy, as γ increases

Analytic self-fields

Different distributions Linear fields in elliptical distributions Charged rings

Poisson solvers Numerically solve $\nabla^2 \phi = -\rho/\mathcal{E}_0$ Spectral and quasi-spectral methods Green Function methods Multigrid methods



Need at least 5-10 particles per cell for reasonable calculation of self-field potential and forces.



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Electromagnetic effects

- Beam self forces as well as beam-environment interactions
- Very time consuming!
- VORPAL movie of JLAB DC gun

QuickTime[™] and a Sorenson Video decompressor are needed to see this picture.

Courtesy P. Stoltz, Tech-X



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Background field descriptions

Field maps, 1D/2D/3D

Taylor series expansion gives off-axis components from derivatives of axial field components. Needs symmetry for good representation.







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Particle loading

- Random number generators how random are they really?
 - System ran()
 - Hammersley sequence
 - Bit-reversal
- Distributions what is a good approximation?
 - Gaussian
 - Parabolic
 - KV
 - Waterbag
- Sampling not good enough, I need to use a 'realistic' distribution
 - Monte Carlo methods
- Noise how quiet does my set need to be, who's listening?
 - Quasi-random sequences to remove particle noise sources
 - 'Quiet load'



Analyzing results

- Standard output
 - Each code will generate a standard set of output based on the run, particle distributions, etc.
 - Emittance (however defined)
 - Beam trajectory, envelope history, . . .
 - There's always some diagnostic that is important to you but which is not included in the standard set
- Particle diagnostics
 - The particle distributions themselves contain all of the available information
 - Get used to performing your own post-processing functions on the raw particle distributions (hopefully, they are part of the output)
 - Slice emittances and mismatches, slice energy spread and energy position correlations, . . .
 - Higher order correlations (x^3 , xx'y, . . .), hidden symmetries



Beam spot/length [mm], Emittance [mm mrad]



How many particles?

- ASTRA simulations, pseudo-analytic (3rd order) fields
- 2D geometry (r-z)
- Spot size, energy, bunch length 2K-5K ۲ Projected emittance, emittance oscillations 10K-25K ۲ Slice emittance 100K • Slice energy spread 500K+ lacksquareLongitudinal µ-bunching instability in 2GeV linac 1G+ ۲ 3D Impact-T



Connecting to Measurements

Eventually, you will want (or will be asked in fairly strong terms) to perform a 'reality check' by benchmarking the results from experiments.

This presents several issues and challenges:

Is there a reasonable model for the beamline that exists? Are the initial conditions known to reasonable accuracy?

What diagnostics exist, and how well can they be modeled with simulation?What measurement uncertainties exist?What instrument resolution exists?



Pepperpot simulation





~100K particles incident at screen ~several hundred particles per 'beamlet'

$$\varepsilon_r^2 = \left\langle r^2 \right\rangle \left\langle r'^2 \right\rangle - \left\langle rr' \right\rangle^2$$



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QuickTime[™] and a TIFF (Uncompressed) decompressor are needed to see this picture.

Courtesy C. Limborg-Deprey



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