Modeling Gas Phase Ultrafast Electron Diffraction

Carlo Santos, Dr. Martin Centurion
Department of Physics and Astronomy, University of Nebraska–Lincoln

Introduction

What is Gas Phase Ultrafast Electron Diffraction (GUED)?

- Technique used for analyzing molecular structural dynamics
- Uses electron bunches to created patterns of molecules

General Particle Tracer (GPT)

- Particle tracking software
- Simulates beam dynamics
- Built-in and custom elements

Purpose of using GPT to model electron motion

- Efficient method for testing adjustable parameters
- Rapid evaluation of theoretical models prior to implementation
- Allows insight into electron motion in unmeasurable regions of GUED

Components

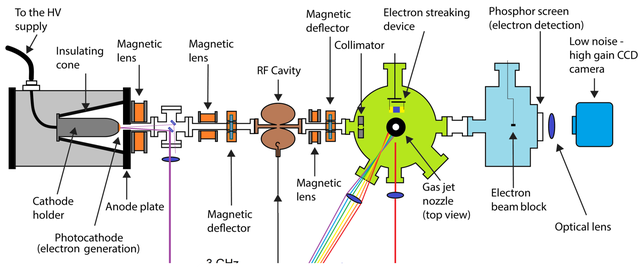


Figure 1. Gas Phase Ultrafast Electron Diffraction Setup [1]

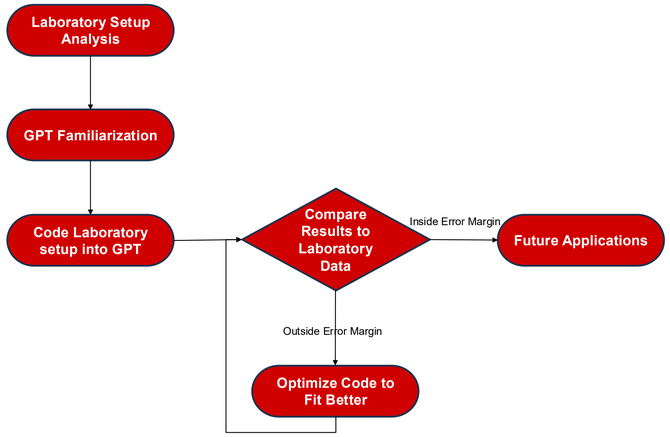
Major Components

- Photocathode
- Magnetic Lenses
- RF Cavity
- Magnetic Deflector

GPT Integration

- Each component has similar elements in GPT
- Each element is used to simulate sections of GUED
- Elements not contained within the software can be coded in manually as custom elements

Methods



- General Particle Tracer simulates particles in snapshots of frames of time
- Using specific snapshots, electron patterns can be compared to the laboratory setup
- Discrepancies between model and setup are continually fixed and optimized within the code

Discussion

- GPT successfully simulated the initial and downstream distribution of electron bunch from photocathode
- Displayed a conical beam after passing through 1 cm electric accelerating field
- Simulation produced 50 μm spot size at photocathode
- Spread and density change over 7 ns confirms GPT's ability to capture temporal resolution over time
- Snapshot tracking helps visualize bunching at any stage

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Results

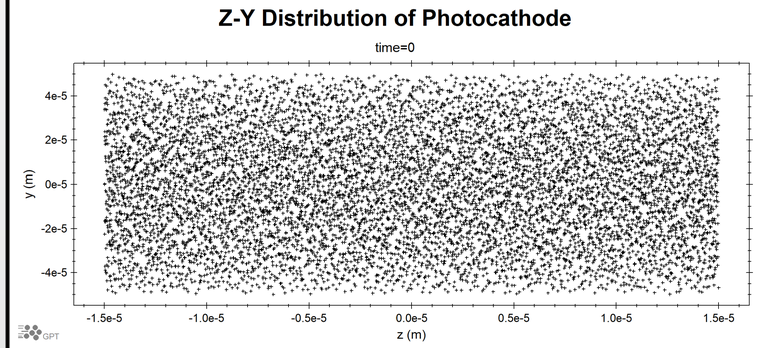

Figure 2. Initial Distribution of electrons at 50μm spot size at photocathode

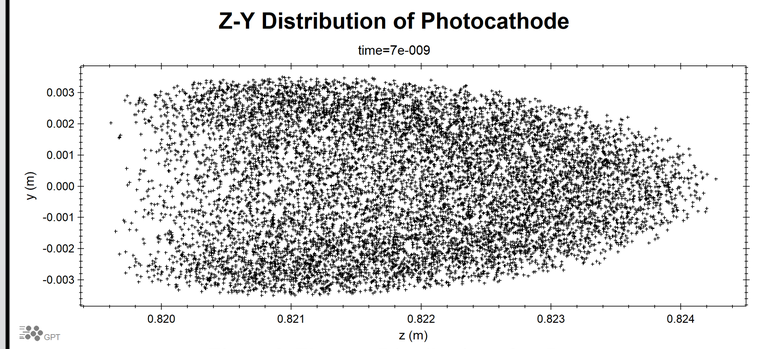

Figure 3. Electron Distribution after 7 ns

Conclusions

- Allows for visualization of beam dynamics in unmeasurable regions
- Efficiently conduct simulations, saving lab time
- Useful for modeling ideal electron bunching prior to adjusting lab setup

Future Work

- Incorporate all components
- Continue to optimize program
- Incorporate 3D field maps for electric and magnetic components

[O. Zandi, Design and Construction of a High-Current Femtosecond Gas-Phase Electron Diffraction Setup, 2017][1]