A High-Precision Emission (HiPE) Computational Model For Ultracold Electron Emission

Alister J. Tencate* and Bela Erdelyi

Department of Physics, Northern Illinois University, DeKalb, IL 60115, USA

*atencate@niu.edu

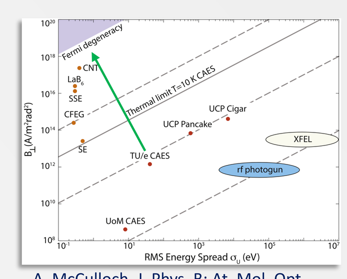
Abstract

The high-intensity, high-brightness and precision frontiers for charged particle beams are an increasingly important focus for study. Ultimately for electron beam applications, including FELs and microscopy, the quality of the source is the limiting factor in the final quality of the beam. It is imperative to understand and develop a new generation of sub-Kelvin electron sources, and the current state of PIC codes are not precise enough to adequately treat this ultracold regime. Our novel computational framework is capable of modelling electron field emission from nanoscale structures on a substrate, with the precision to handle the ultracold regime. This is accomplished by integrating a newly developed Poisson integral solver capable of treating highly curved surfaces and an innovative collisional N-body integrator to propagate the emitted electron with prescribed accuracy. The electrons are generated from a distribution that accounts for quantum confinement and material properties and propagated to the cathode surface. We will discuss the novel techniques that we have developed and implemented and show emission characteristics for several cathode designs.

Introduction

The ultimate lower limit in beam emittance is governed by the quantum degeneracy limit

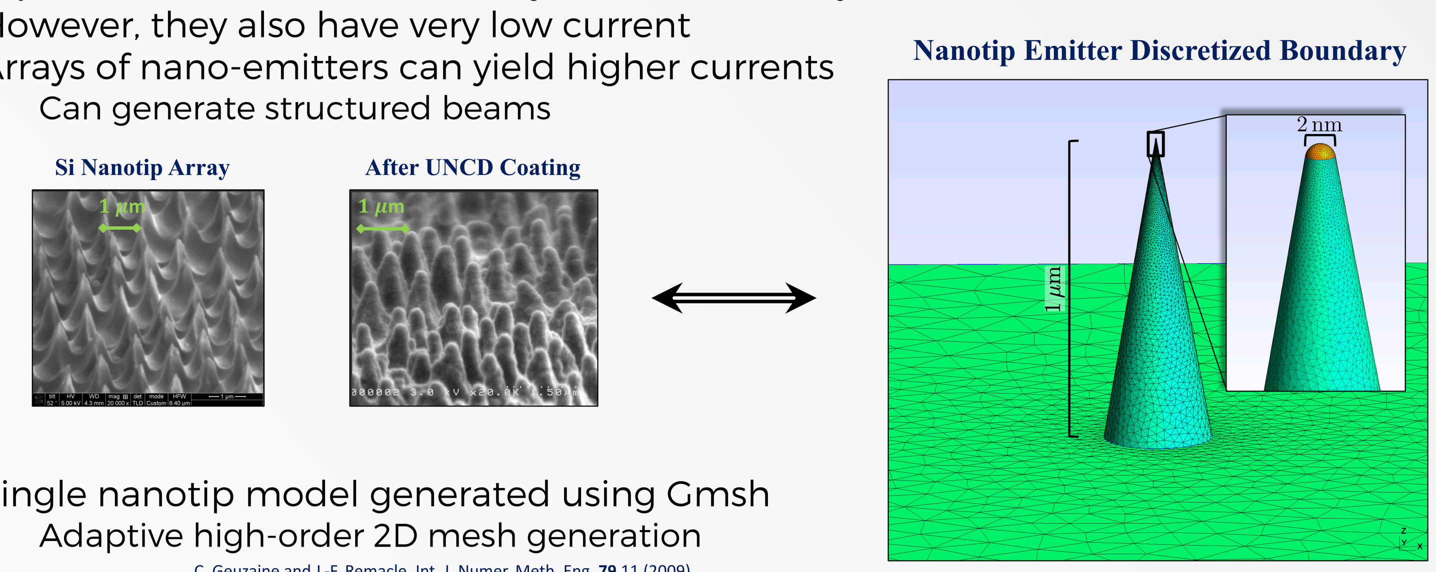
- Ultracold electron sources seek high brightness and low emittance
- Applications:
  - Injectors for free electron lasers
  - High-intensity accelerator sources
  - Ultrafast electron microscopy/diffraction
    - High spatial resolution with short time scales



A. McCulloch, J. Phys. B: At. Mol. Opt. Phys. **49** 164004 (2016)

Sharp-tip (nanoscale) emitters have yielded extremely low emittances

- However, they also have very low current
- Arrays of nano-emitters can yield higher currents
  - Can generate structured beams



- Single nanotip model generated using Gmsh
  - Adaptive high-order 2D mesh generation

C. Geuzaine and J.-F. Remacle, Int. J. Numer. Meth. Eng. **79** 11 (2009).

Large arrays of nanotip emitters present a significant computational challenge

- Standard PIC/FEM modelling tools are inefficient
  - Needle-shaped tip (nanometer scale variation)
  - Array of hundreds of tips (100s of micrometers)
  - Similarly significant range in relevant time scales

→ Develop a High-Precision Emission (HiPE) computational model
  - Meet accuracy and efficiency requirements

Code Modules and Integration

Programmed in Fortran-based COSY Infinity

- Robust suite of beam physics routines/procedures
  - Map analysis and manipulation
  - Electromagnetic and optical accelerator components
- Language-level differential algebra (DA) implementation
  - Map analysis and manipulation

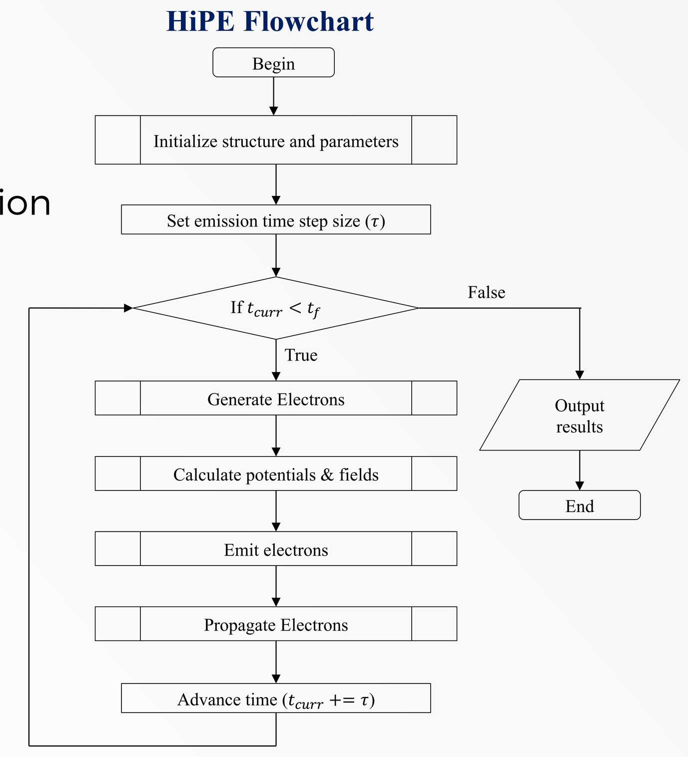
M. Berz and K. Makino, Michigan State University, Aug. 2017.

Three fundamental physical processes to consider:

- Initial electron distribution and transport to surface
- Electron transmission through boundary potential
- Propagation of emitted electrons
  - Tracked to evaluation plane (constant external field)

- HiPE dynamics governed by τ
  - Constant user-specified time step parameter

HiPE Flowchart



Initial Electron Distribution and Transport

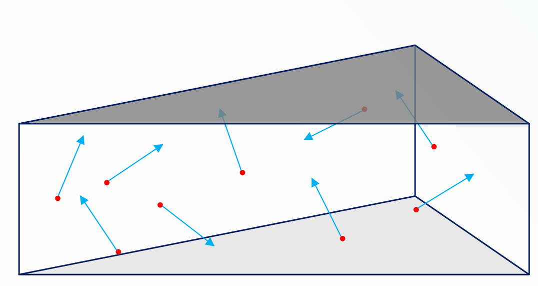
The electron distribution is dependent on the geometric/material properties of the cathode

- Electron density (n) given by Fermi-Dirac statistics and the density of states
  - Electron distribution within a layer δ_p under a triangular surface element

$$\mathcal{F}(E) = \frac{1}{\exp[\frac{E-\mu}{k_B T}]+1}$$

$$g(E) = \frac{(2m^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E-E_c}$$

$$n(E) = g(E)\mathcal{F}(E)$$



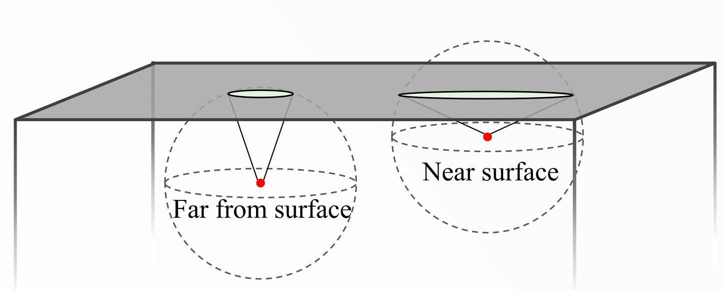
$\delta_p = \tau v_{max}$

- Sampling efficiently by factoring the momentum angle distribution
  - Probability that an electron initially at a depth of z_i will encounter the surface boundary:

$$P(E) = \frac{1}{2} - \sqrt{\frac{m z_i^2}{8E\tau^2}}$$

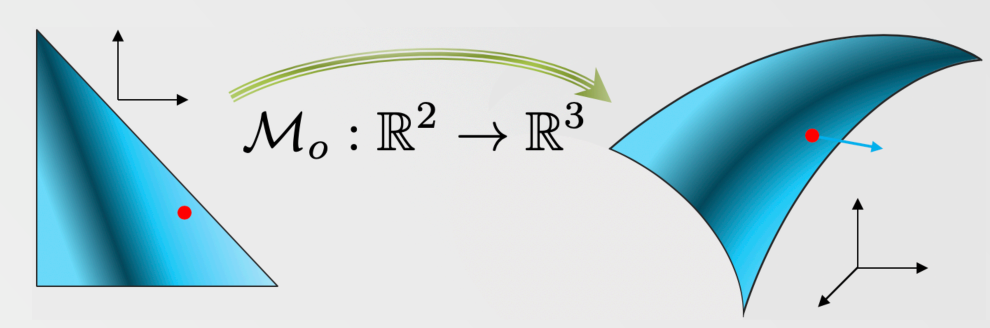
- Only sample N relevant electrons from $n(E)$

$$N = \int_0^\infty P(E)n(E)\delta_p \tau \mathrm{d}E$$



Parallelizability by parametric mapping from unit triangle to surface element

- Electrons are generated and transported to the surface of the 2D right unit triangle
  - Generalize and efficiently parallelize
- $\mathcal{M}_o$ is a polynomial map of order o formed using the DA framework in COSY
  - Yields both the points and the surface normals of the boundary element

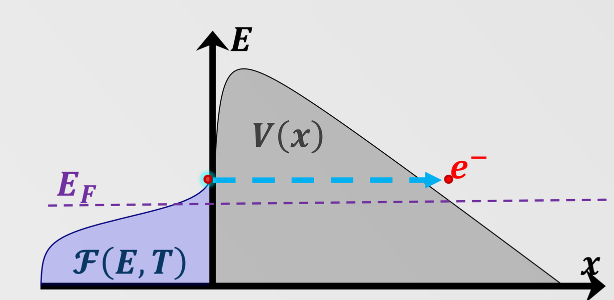


Electron Emission and Poisson Solver

Transmission coefficient gives probability that electron tunnels through the surface barrier

- Determined by the semi-classical 1D WKB method
- Depends on the external electric potential

$$\mathrm{T}(E) = \exp\left[-\frac{2}{\hbar}\int\sqrt{2m(V(x)-E)}\mathrm{d}x\right]$$



Potentials and fields calculated using PISCS

- Poisson Integral Solver with Curved Surfaces

A. Gee, PhD dissertation, Northern Illinois University, 2018.

- Utilizes an adaptive fast multipole method to accurately/efficiently solve the N-body force problem

S. Abeyratne, A. Gee, and B. Erdelyi, *Commun. Nonlinear. Sci.* **72** (2019).

Propagation of Electrons Utilizing SIMO and PISCS

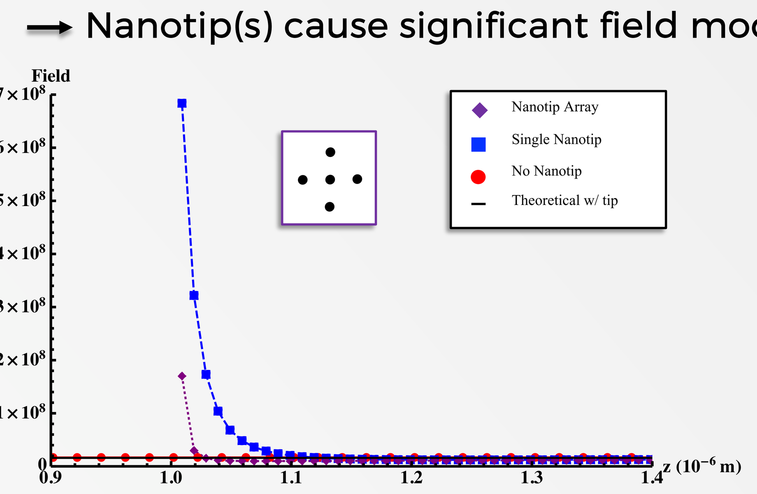
Dynamics of electron beam near nanotip array with SIMO integrator

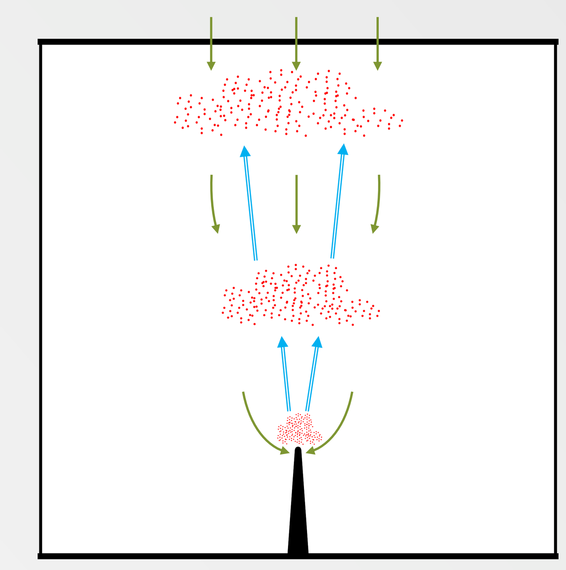
- Accurate and efficient collisional N-body numerical integrator

A. Al Marzouk and B. Erdelyi, *SIAM J. Sci. Comput.*, **40** 6 (2018).

- Functional form of external fields given by PISCS
  - Series expansion using DA

→ Nanotip(s) cause significant field modification





Conclusion

Simulating electron emission from a nanotip array is a significant computational challenge!

- Important physical processes scale from
  - $\mathcal{O}$(nm) to $\mathcal{O}$(> 100 μm) – Sharp tip to source size
  - $\mathcal{O}$(< fs) to $\mathcal{O}$(ns) – Close collisions to travel time to evaluation plane

HiPE is designed to efficiently meet these accuracy requirements

- High-order polynomial surface parametrization
- Particle-level model of electron emission
- Accurate computation of electric potentials and fields (PISCS)
  - Factoring in the highly curved surface
- Accurate beam dynamics near cathode (SIMO and PISCS)
  - takes into account all particle-particle collisions, including close encounters

PISCS, the FMM, SIMO and other scripts are available for download with documentation and examples!

- Expect a working version of HiPE with documentation and examples soon

Beam Physics Code Repository
https://www.niu.edu/beam-physics-code/projects/index.shtml

Acknowledgements

The author appreciatively acknowledges NAPAC2019 for a Student Grant award. Additional thanks is due to the Department of Physics, the College of Liberal Arts and Sciences, and the Graduate School at Northern Illinois University for supplemental travel funding.

This work was supported by the National Science Foundation (NSF) under Grant PHY-1535401 with Northern Illinois University.

NAPAC2019
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