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A High-Order Fast Boundary Element Method with Near-Boundary Stability for Field Emission from Nanoscale Structures

Alister J. Tencate* and Béla Erdélyi

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

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Abstract. Advancing electron beam applications require pushing toward the quantum degeneracy limit. Nanoscale structured cathodes are a promising electron source for this regime, but the numerical tools for studying these designs remain limited. A previous paper detailed the implemented of a flat-panel fast-multipole-accelerated boundary element method, which solves the relevant Poisson problem. However, flat panels are inadequate and inefficient for representing curved surfaces at the high precision necessary for many applications. Additionally, the boundary element method has an established numerical instability when evaluated near the domain boundary. To resolve this, a general high-order curvilinear element interpolation and modified quadrature method is developed utilizing a differential algebraic mapping for greater accuracy in the boundary surface representation. The boundary instability effect is mitigated by devising local corrections to the quadrature scheme in the form of Cartesian Taylor expansions. This approach is suitably general, requiring only small modifications for application to other kernels, and can easily be incorporated into a fast multipole accelerated framework. The refined algorithm is evaluated with respect to both accuracy and efficiency using several analytic structures and the performance capacity is highlighted by the capability of accurately determining the field enhancement factor for a single nanotip electron cathode.

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Key words: Quadrature by expansion, high-order boundary interpolation, fast-multipole accelerated boundary element method, differential algebraic framework.

1 Introduction

Many applications pushing the high-intensity, high-brightness, and precision frontiers for charged particle beams require low emittance sources. Simulating particle emission

*Corresponding author. *Email addresses:* atencate@niu.edu (A. J. Tencate), berdelyi@niu.edu (B. Erdélyi)

from these cathodes presents unique numerical challenges, especially for cathodes comprised of nanoscale structures. A cathode consisting of an array of sharp nanotip emitters has been proposed as a potential candidate for increasing the current while maintaining the low emittance found in single nanotip transmission electron microscopy devices [1–4]. In order to evaluate these proposed designs, precise numerical models must be capable of handling widely varying length scales and accurately computing the electric potential distribution near the cathode surface in the presence of charged particles.

Recently, we detailed the development of a three dimensional Poisson solver for a collection of charged particles within complicated electromagnetic structures, called PISCS [5]. A charged particle beam within a bounded structure yields a Poisson problem. The linearity of the Laplacian enables the decomposition of this system into a bounded Laplace problem and a boundaryless Poisson problem [5],

$$\left.\begin{aligned} \nabla^2\tilde{\psi}(\mathbf{x}) &= 0 \\ \nabla^2\varphi(\mathbf{x}) &= \frac{\rho(\mathbf{x})}{\varepsilon_0} \end{aligned}\right\} \quad \text{for } \mathbf{x}\in\Omega;$$
$$\left.\begin{aligned} \tilde{\psi}(\mathbf{y}) &= \tilde{g}(\mathbf{y}) \\ &\text{or} \\ \frac{\partial\tilde{\psi}}{\partial n_y}(\mathbf{y}) &= \tilde{h}(\mathbf{y}) \end{aligned}\right\} \quad \text{for } \mathbf{y}\in\Gamma, \tag{1.1}$$

where $\Omega\subset\mathbb{R}^3$ is a bounded domain with a uniformly continuous boundary Γ, and the full solution is given by $\psi=\tilde{\psi}+\varphi$. The modified boundary conditions $\tilde{g}$ or $\tilde{h}$ are given by,

$$\begin{aligned} \tilde{g}(\mathbf{y}) &= g(\mathbf{y})-\varphi(\mathbf{y}), \\ \tilde{h}(\mathbf{y}) &= h(\mathbf{y})-\frac{\partial\varphi}{\partial n_y}(\mathbf{y}), \end{aligned} \tag{1.2}$$

where the applied Dirichlet boundary conditions g (or Neumann h) are fully specified on Γ. The Neumann problem is only unique up to a constant, so the final solution will require matching the potential to a known value. To minimize distortion when there is a gradient in the potential, it is best to fit the solution based on an average of values from a sampling of points on the boundary.

The source term ρ describes a beam of N point-like particles

$$\rho(\mathbf{x}) = \sum_{i=1}^{N} q_i\delta(\mathbf{x}-\mathbf{x}_i), \tag{1.3}$$

where q_i denotes the charge and $\mathbf{x}_i$ the position of the i-th particle; the well-known solution is given by [Equation (1.17) using (1.6) in [6]]

$$\varphi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0}\sum_{i=1}^{N}\frac{q_i}{\|\mathbf{x}-\mathbf{x}_i\|}. \tag{1.4}$$